

# Biological and Environmental Research

## Program Mission

For over 50 years the Biological and Environmental Research (BER) program has been advancing environmental and biomedical knowledge that promotes national security through improved energy production, development, and use, international scientific leadership that underpins our nation's technological advances, and environmental research that improves the quality of life for all Americans. BER supports these vital national missions through competitive and peer-reviewed research at National Laboratories, universities, and private institutions. In addition, BER develops and delivers the knowledge needed to support the President's National Energy Plan, provides the science base in support of the Energy Policy Act of 1992, and works cooperatively with DOE's national security programs to develop tools to combat terrorism.

## Strategic Objective

- SC3:** By 2010, develop the basis for biotechnology solutions for clean energy, carbon sequestration, environmental cleanup, and bioterrorism detection and defeat by characterizing the multiprotein complexes that carry out biology in cells and by determining how microbial communities work as a system; and determine the sensitivity of climate to different levels of greenhouse gases and aerosols in the atmosphere and the potential consequences of climate change associated with these levels by resolving or reducing key uncertainties in model predictions of both climate change that would result from each level and the associated consequences.
- SC7:** Provide major advanced scientific user facilities where scientific excellence is validated by external review; average operational downtime does not exceed 10% of schedule; construction and upgrades are within 10% of schedule and budget; and facility technology research and development programs meet their goals.

Progress toward accomplishing these Strategic Objectives will be measured by Program Strategic Performance Goals, Indicators and Annual Targets, as follows:

## Program Strategic Performance Goals

**SC3-1:** Determine, compare, and analyze DNA sequences of microbes and other organisms that will underpin development of biotechnology solutions for clean energy, carbon sequestration, environmental cleanup, and bioterrorism detection and defeat. (Life Sciences, Environmental Remediation, and Medical Applications and Measurement Science subprograms)

### Performance Indicator

Base pairs of DNA sequenced per year.

### Performance Standards

As discussed in Corporate Context/Executive Summary.

### Annual Performance Results and Targets

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
<p>By the end of FY 2001, the DOE Joint Genome Institute (JGI) completed the sequencing and submission to public databases of an additional 100 million finished and 250 million high quality draft base pairs of DNA, including both human and model organisms (e.g., the mouse) as part of the Human Genome Program. (SC2-1) [Exceeded goal]</p>	<p>By the end of FY 2002, the DOE Joint Genome Institute will complete the high quality DNA sequence of human chromosomes 16 and 19 and produce 6 billion base pairs of DNA sequence from model organisms (e.g., mouse, Fugu, and Ciona) to help understand the human sequence as part of the Human Genome Program. (SC3-1)</p>	<p>Complete the high quality DNA sequence of human chromosome 5. (SC3-1)</p> <p>Increase the DNA sequencing capacity of the DOE Joint Genome Institute (JGI), with no additional funding, to approximately 8 billion base pairs of DNA sequence per year, a 100% increase in the projected capacity over FY 2001. Establish at least 30 diverse collaborations for high throughput DNA sequencing with scientists outside the JGI important for Genomics and Genomes to Life research. (SC3-1)</p>
<p>Completed the genetic sequencing of three additional microbes that produce methane or hydrogen from carbonaceous sources and that could be used to sequester carbon as part of the Microbial Genomics and Carbon Sequestration programs. (SC2-1) [Exceeded goal]</p>	<p>Produce draft DNA sequence of more than 30 microbes that cover a range of functional relevance to DOE's life and environmental sciences and security missions - including carbon sequestration, environmental cleanup, bioremediation, and bioterrorism. (SC3-1)</p>	<p>Produce draft DNA sequences of more than 30 microbes vital to future U.S. energy security and independence, carbon sequestration, and environmental cleanup. (SC3-1)</p>

**SC3-2:** Establish the scientific foundation for determining a safe level of greenhouse gases and aerosols in the atmosphere by resolving or reducing key uncertainties in predicting their effects on climate, and provide the foundation to predict, assess and mitigate potential adverse effects of energy production and use on the environment. (Climate Change Research subprogram)

**Performance Indicator**

Climate model resolution.

**Performance Standards**

As discussed in Corporate Context/Executive Summary.

**Annual Performance Results and Targets**

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
<p>Conducted five Intensive Operations Periods (IOPs) on schedule at the Atmospheric Radiation Measurement (ARM) Southern Plains site in Oklahoma. Obtained data from second station on the North Slope of Alaska, and made operational the third station in the Tropical Western Pacific on Christmas Island on schedule and within budget in accordance with program plan. (SC2-1) [Met goal]</p>	<p>Develop and test a fully-coupled atmosphere-ocean-land-sea ice climate model that has twice the spatial resolution of coupled models available in 2000 as part of Climate Modeling and Prediction research. Support multi-disciplinary teams of scientists at multiple institutions using DOE supercomputers to perform model simulations, diagnostics, and testing. (SC3-2)</p>	<p>Improve the precision of climate models by delivering a more realistic cloud submodel that reduces the uncertainty in calculations of the atmospheric energy budget by 10 percent and by increasing the spatial resolution of the atmospheric and ocean and sea ice submodels to 1.4 degrees (about 150 Kilometers) and approximately 0.7 degrees (about 75 Kilometers), respectively, for the fully coupled climate model. (SC3-2)</p>

**SC7-3:** Manage all BER facility operations and construction to the highest standards of overall performance, using merit evaluation with independent peer review. (Life Sciences, Environmental Remediation subprograms).

**Performance Indicator**

Percent on time/on budget, percent unscheduled downtime.

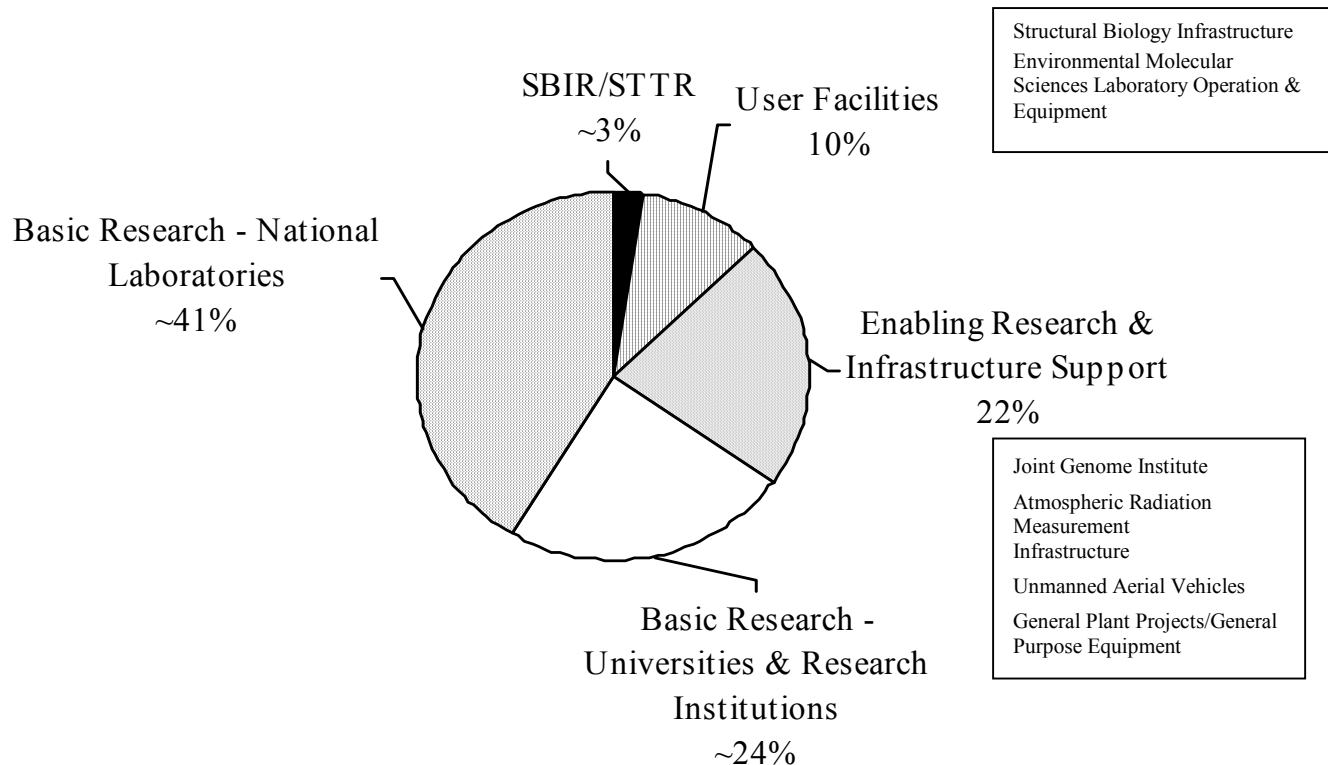
**Performance Standards**

As discussed in Corporate Context/Executive Summary.

**Annual Performance Results and Targets**

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
<p>Keep within 10 percent of cost and schedule milestones for upgrades and construction of scientific user facilities, initiate commissioning of the protein crystallography Structural Biology User Station at the Los Alamos National Laboratory and initiate construction of the Center for Comparative and Functional Genomics at Oak Ridge National Laboratory. [Met Goal]</p>	<p>Keep within 10 percent of cost and schedule milestones for upgrades and construction of scientific user facilities; begin acceptance testing of the new high performance computer at the Environmental Molecular Sciences Laboratory at the Pacific Northwest National Laboratory; continue construction of the Center for Comparative and Functional Genomics at Oak Ridge National Laboratory. (SC7-3)</p>	<p>Keep within 10 percent of cost and schedule milestones for upgrades and construction of scientific user facilities; begin operation of the new high performance computer at the Environmental Molecular Sciences Laboratory at the Pacific Northwest National Laboratory; complete construction of the Center for Comparative and Functional Genomics at Oak Ridge National Laboratory. (SC7-3)</p>
<p>Maintain and operate the BER scientific user facilities so the unscheduled downtime on average is less than 10 percent of the total scheduled operating time. [Met Goal]</p>	<p>Maintain and operate the BER scientific user facilities so the unscheduled downtime on average is less than 10 percent of the total scheduled operating time. (SC7-3)</p>	<p>Maintain and operate the BER scientific user facilities so the unscheduled downtime on average is less than 10 percent of the total scheduled operating time. (SC7-3)</p>

To accomplish the BER Program strategic goals, the BER budget request for FY 2003 is \$504,215,000, including support for basic research, scientific user facility operations, and enabling research and infrastructure support. In addition, the program includes funding for the Small Business Innovation Research (SBIR) and Small Business Technology Transfer program (STTR).



#### PROGRAM REVIEW, PEER REVIEW, AND USER FEEDBACK

Effective program review, peer review, and user feedback are critical tools for BER to measure performance of research programs, research projects, and user facilities. The quality and scientific relevance of the BER program and its individual research projects are maintained by rigorous peer reviews conducted by internationally recognized scientific experts. The criteria for determining scientific quality and relevance include scientific merit, appropriateness of the proposed approach and requested level of funding, and qualifications of the principal investigator. BER expects the highest quality research and, when necessary, takes corrective management actions based on results of the reviews. A measure of the quality of the BER research is the sustained achievement in advancing scientific knowledge. This is demonstrated by the publication of research results in the leading refereed scientific journals pertinent to BER-related research fields, by invited participation at national and international scientific conferences and workshops, and by honors received by BER-supported researchers. BER regularly compares its programs to the scientific priorities recommended by the Biological and Environmental Research Advisory Committee (BERAC), and by the standing committees created by the Office of Science and Technology Policy.

The BER program benefits from a diversity of program reviews. This is particularly the case for BER program elements that are components of international research endeavors, e.g., the International Human Genome Project and the U.S. Global Change Research Program. In addition to panel reviews used to evaluate and select individual projects and programmatic reviews by the chartered BERAC, BER evaluates its programs using interagency (and international) review bodies and by Boards and Committees of the National Academy of Sciences.

BER goes one step further in conducting program reviews. Panels of distinguished scientists are regularly charged with evaluating the quality of individual programs and with exploring ways of entraining new ideas and research performers from different scientific fields. This strategy is based on the conviction that the most important scientific advances of the new century will occur at the interfaces between scientific disciplines, such as biology and information science. Groups like JASON and The Washington Advisory Group (WAG), involving physicists, mathematicians, engineers, etc., are among the organizations that study BER program elements, such as the Atmospheric Radiation Measurement (ARM) program, climate change prediction activities, the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), and the Human Genome program. The BER program is ideally positioned to facilitate and foster interactions between the physical sciences and the life sciences and aggressively pursues every opportunity to enhance the interface between the two scientific domains.

BER facility operations are also monitored by peer reviews and user feedback. BER manages these facilities in a manner that meets user requirements as indicated by achieving performance specifications while protecting the safety of the workers and the environment. Facilities are operated reliably and according to planned schedules. Facilities are also maintained and improved to remain at the cutting edge of technology and scientific capability.

The reviews and user feedback are incorporated as BER plans for the future needs of DOE research in the life and environmental sciences. This includes: planning for future directions, opportunities, and initiatives within the BER research portfolio; maintaining the flexibility to quickly move into promising new areas; contributing to the health of the educational pipeline in critical subfields and disciplines; planning for upgrades at existing facilities to expand the research capabilities or operational capacity; ensuring the proper balance between facilities and research; and planning for future facilities necessary to advance the science in areas relevant to BER's mission in close collaboration with the research community.

## BER LEADERSHIP AND UNIQUE ROLES

The BER program fills a broad range of unique roles for the Department and the national and international scientific communities including:

- Manage research on microbes for energy, the environment, and national security and work with the Advanced Scientific Computing Research program to develop the computational methods and capabilities needed to advance understanding of complex biological systems, predict their behavior, and use that information to address DOE needs.
- Provide the facilities, instrumentation, and technology needed to (1) characterize the multiprotein complexes that result in microbial products and processes of use to DOE, and (2) determine the functional repertoire of complex microbial communities that can be used to address DOE needs.
- Develop cutting edge technologies, facilities, and resources, including animal models, for the Human Genome Project.

- Provide world leadership in low dose radiation research.
- Provide world-class structural biology user facilities and unique computational and experimental structural biology research emphasizing protein complexes involved in recognition and repair of DNA damage and remediation of metals and radionuclides.
- Provide world leadership in ground-based measurement of clouds and atmospheric properties to resolve key uncertainties in climate change, through the Atmospheric Radiation Measurement (ARM) program.
- Develop advanced predictive capabilities using coupled climate models on massively parallel computers for decade-to-century long simulations of climate change.
- Support fundamental research on carbon sequestration to develop technologies that enhance the uptake of carbon in terrestrial and ocean ecosystems.
- Provide world-class scientific user facilities for environmental and climate change research.
- Provide world leadership in radiopharmaceutical development for wide use in the medical and research communities.
- Maintain world leadership in detector development for medical and biological imaging.
- Enable interdisciplinary teams of scientists to use the unique resources in physics, chemistry, material sciences, and biology at the National Laboratories to develop novel medical applications.
- Manage the Environmental Management Science Program (EMSP) in consultation with the Office of Environmental Management (EM) to identify and select the appropriate fundamental research activities.
- Ensure that the rights and welfare of human research subjects at the Department are protected while advances in biomedical, environmental, nuclear, and other research lead to discoveries that benefit humanity.

## **Significant Accomplishments and Program Shifts**

### SCIENCE ACCOMPLISHMENTS

#### Life Sciences

- *Human DNA Sequence Published* - Capping what may be one of the greatest scientific achievements of all time, the draft human DNA sequence was published in the February 15/16, 2001 issues of the journals *Nature* and *Science*. DOE initiated this monumental research project, sequenced human chromosomes 5, 16, and 19, and contributed many of the fundamental technologies and resources. Both the human DNA sequence and high throughput DNA sequencing capabilities, especially as applied to microbes, contribute to the identification of genetic factors that increase individual human susceptibility to radiation and other energy-related materials and to the use of microbes and microbial communities to solve challenges in carbon sequestration, clean energy, environmental cleanup, and national security.
- *Understanding Human Chromosome 19 by Studying the Mouse* - Interpreting the recently completed human DNA sequence and understanding the role each gene plays in human development, health and susceptibility is one of the next major challenge in biology. Identifying all the components of each human gene is made easier by comparing the human DNA sequence with the comparable

sequence in the mouse, sequences that have been remarkably conserved by evolution. The JGI has sequenced more than 42 Megabases (Mb) of the mouse genome that codes for genes related to those found on human chromosome 19. For a particular gene-rich region of human chromosome 19, called HSA 19, research to date has shown that direct counterparts of virtually all known genes in the HSA 19 region are found in the mouse. In particular, these initial comparisons identified both new genes and candidate regulatory regions that had not been found with “gene-finding” software.

- *Sequencing the Pufferfish to Understand the Human Genome* - Scientists searching the human genome for genes and their on/off switches will soon have a valuable new resource courtesy of the Japanese delicacy known as Fugu, or the pufferfish. Evolution has conserved many of the DNA sequences that code for genes or their regulatory sequences. Comparisons of genome sequences between species are, therefore, an effective and efficient means of finding new genes and gene regulatory (controlling) elements. The Fugu genome, is 8-fold more compact than the human genome, making it even more cost-effective for these comparisons than yeast, fly, worm, and mouse. In FY 2001, DOE’s Joint Genome Institute, together with its international partners, determined more than 90-percent of the Fugu genome sequence and made it available in an accessible database.
- *DOE Investments in Structural Biology Make Big Payoffs* - Understanding the three dimensional structure of proteins is an important step in understanding how the information contained in genes is put into action. This knowledge has important applications in medicine, clean energy production, carbon sequestration, and environmental cleanup since proteins make biology “happen” whether in people or microbes. DOE investments in structural biology research, at user facilities at synchrotron light sources, and in the technologies for speeding the determination of protein structure have enabled the National Institute of General Medical Sciences at the National Institutes of Health to make a large investment (over \$25,000,000 in FY 2001) in pilot projects for the NIH’s new Protein Structure Initiative to develop high throughput methods for determining protein structure. Five of the seven initial pilot projects include partners from DOE Laboratories and nearly all are using DOE user facilities.
- *Approaching High Throughput Proteomics* - Pacific Northwest National Laboratory has developed a “next generation” instrument for quantitative high throughput proteomic studies of microorganisms that also holds promise for studies of higher organisms including mouse and human. Initial studies with the highly radiation resistant microorganism *Deinococcus radiodurans*, now being extended to *Shewanella oniedensis*, (both important in bioremediation and waste cleanup), gave precise, proteome-wide measurements of changes in protein abundances based on the use of atomic mass tags and a stable-isotope labeling method, thus, allowing effective comparison of the proteome of an organism under two different experimental conditions.
- *Record Breaking Year of Microbial DNA Sequencing* - In FY 2001 the DOE Joint Genome Institute (JGI) sequenced over 20 different microbial genomes. The high draft sequence quality enabled 95% of the genes in these organisms to be identified. This is the largest microbial data set produced in such a small period of time, making the JGI one of the largest producers of microbial genomic sequence. The microbes cover a range of functional relevance to DOE’s life and environmental sciences mission - from carbon sequestration to environmental, bioremediation, and medical relevance. Each microbe had a scientific “champion” to ensure rapid and public dissemination and use of the data. This draft sequencing effort is part of an ongoing scientific test to determine the most effective way to generate and disseminate the largest amount of useful DNA sequence information to the scientific community in the shortest, most cost effective manner.



- *White Rot Fungus Sequenced* - In FY 2001, the JGI completed the draft DNA sequence of the 30 Mb White rot fungus, *Phanerochaete chrysosporium*. This is one of the first fungal genomes to be sequenced and is a landmark in the use of whole genome shotgun strategies and the testing of the JGI's genome assembler software. The white rot fungus genome is very important to current research in the areas of biomass conversion, carbon sequestration, and cellulose and lignin digestion as well as PCB detoxification.
- *Resolving A-Bomb Dosimetry After More than 50 Years* – BER, working with DOE's Office of Environment, Safety and Health; National Research Council; and RERF (Radiation Effects Research Foundation) is resolving A-bomb dosimetry after more than 50 years. This effort was conducted in response to a directive from Congress to the BER program. Standards for protecting people from exposure to ionizing radiation are based, in large part, on analyses of the survivors of the atomic bombs in Hiroshima and Nagasaki. However, these analyses have large uncertainties due to uncertainties in the estimated doses of radiation received by the survivors. New technologies for measuring irradiated materials and greatly increased computational capabilities are now leading to the development of a new dosimetry system for A-bomb survivors that will be completed in early 2002. This new A-bomb dosimetry will be used for the development of future radiation protection standards, important both for future uses of nuclear energy and for ongoing clean up of contaminated DOE sites.

#### Climate Change Research

- *Improvements in Measurements and Modeling of Atmospheric Radiation Improves Weather Forecasts* - Through improvements in measurement techniques and related climate model radiation codes, the ARM program has improved the agreement between measured and modeled instantaneous clear sky infrared fluxes from 20 Watts/m<sup>2</sup> to 5 Watts/m<sup>2</sup>. The inclusion of the advanced radiation code into climate models has resulted in a 7 percent improvement in the usefulness of weather forecasts by extending the forecast period and reducing the computation time required to produce the forecasts.
- *Consistency Documented Between Observed Temperature Changes in the Atmosphere and Ocean and Model Simulated Temperature Changes* - The Parallel Climate Model (PCM), a collaborative climate modeling effort supported by BER at the National Center for Atmospheric Research and Los Alamos National Laboratory, with contributions from several other DOE National Laboratories and academic institutions, was applied to the problem of identifying whether a greenhouse-gas climate signal exists in the observational climate record. BER-supported researchers at Scripps Institution of Oceanography compared two ensembles of PCM simulations of the last 300 years. The first ensemble was a series of simulations that included observed increases in greenhouse gas and sulfate aerosol concentrations resulting from anthropogenic activities. The second ensemble was a series of "control runs" identical to the first series, except that the increases of greenhouse gas and sulfate aerosol concentrations were excluded. The results show that the simulated regional temperature changes in both the atmosphere and the ocean were statistically consistent with the observed data, the first time that a model has demonstrated the ability to realistically simulate both the atmosphere and the ocean. The analysis further revealed a statistically significant pattern of temperature differences between the forced simulations and the control run ensemble that can be attributed to human-induced climate change.
- *Understanding of Complex Pollution Phenomena Advanced* - Data from the Texas Air Quality Study (TexAQS 2000) has provided new information on the relative importance of emissions from

refineries and other sources of ozone and aerosols and the recirculation of polluted air from land and sea breezes in causing violations in ozone and particulate air quality standards in the Houston area. The research was an interagency effort supported by DOE, EPA, NOAA, NSF, TVA, NASA, the Texas Natural Resources Conservation Commission, and the Greater Houston Partnership. Information from this study is being provided to Texas authorities developing air quality improvement plans. Advances in the science are also being incorporated in predictive and assessment models that can then be applied to other urban areas.

- *Assessment of "Background" Sources of Ozone in Urban Areas* - Research using numerical chemistry and atmospheric transport models has improved our understanding of the processes that govern tropospheric ozone, other oxidants, and aerosols on urban, regional, and global scales. A major question is whether horizontal transport by winds over regional distances, up to about 1000 kilometers, can substantially influence concentrations of these pollutants in U.S. metropolitan areas. Evaluation of data from recent field studies showed that ozone produced in southern California might be carried to the Phoenix area, thus altering the effectiveness of potential localized controls on energy-related emissions that contribute to oxidant formation where the current urban background concentration is about 40 parts per billion by volume (ppbv). Surface ozone concentrations can be elevated over this background by 5 to 25 ppbv, usually in episodic events by this regional scale transport. In addition, transport of ozone from the stratosphere can increase surface ozone by 10 ppbv or more near the surface.
- *AmeriFlux Network Increased to 40 Sites for Measuring N. American Terrestrial Carbon Sink* - The AmeriFlux network where net carbon dioxide (CO<sub>2</sub>) exchange between the atmosphere and ecosystems across North America is measured, increased to 40 locations. The systematic net carbon dioxide exchange measurement offers one approach for estimating how much excess carbon dioxide from fossil fuel combustion is sequestered by terrestrial ecosystems. Over the past 3 years, annual net production or carbon gain of the instrumented forest sites ranged from 2 to 4 metric tons per hectare. For example, the carbon gain by deciduous forest ecosystems averages 6 grams of carbon per square meter per day. Net production generally increased with growing season length, which means that early onset of the growing season, or longer growing seasons associated with future climate changes can theoretically lead to more carbon sequestration. Related scientific research also determined that cloudiness leads to more efficient photosynthetic use of light by the plants to fix carbon. Web-based AmeriFlux data are disseminated to the scientific community by the Carbon Dioxide Information and Analysis Center where, in 2000, over 30,000 inquiries from 24 countries were recorded on the web site. In addition, the network is providing both high quality, real-time micrometeorological data for modeling ecosystem processes, and ground-truth plant productivity data for a NASA satellite platform designed to provide estimates of global ecosystem productivity.
- *Novel Ecological Results Obtained from Elevated-Carbon Dioxide Field Experiments* - Recent BER-sponsored Free-Air Carbon Dioxide Enrichment (FACE) field experiments that address DOE's mission to ensure that energy systems are environmentally sustainable have led to discoveries about ecosystem responses to future increases in atmospheric carbon dioxide levels resulting from fossil fuel combustion. In the southwestern U.S., a 50% increase in atmospheric carbon dioxide stimulated growth and seed production of an invasive annual grass species to a greater extent than native annual plants. This indicates that rising atmospheric carbon dioxide may favor exotic annual grasses, which might accelerate the fire cycle and reduce biodiversity in arid ecosystems. In a northern-U.S. FACE experiment, more diverse plant communities were found to respond more favorably to elevated carbon dioxide than less diverse communities, suggesting that biodiversity

losses could significantly affect how terrestrial ecosystems will respond to increasing atmospheric carbon dioxide. In a southeastern loblolly pine plantation in which 16 year old loblolly pines were exposed to elevated carbon dioxide, growth and carbon sequestration by this forest ecosystem were enhanced most when the poorest quality sites received both carbon dioxide and nutrient (nitrogen) amendments. The trees exposed to elevated carbon dioxide alone (55% above ambient) reached reproductive maturity at least two years sooner than trees exposed to the ambient carbon dioxide concentration. Elevated carbon dioxide also resulted in a disproportionate allocation of carbon to cones and seeds compared to tree stems (wood). The responses have implications for management of future forests regarding rotation intervals and selection of species grown for commercial purposes.

- *Fate of Injected Carbon Dioxide in the Deep Ocean Modeled* - LLNL researchers at the DOE Ocean Carbon Sequestration Consortium published a numerical simulation of the distribution of the relative carbon dioxide concentrations in the ocean resulting from a continuous 20-year injection of carbon dioxide at 1700 meters depth near Cape Hatteras, North Carolina. This simulated scenario showed that the injected carbon dioxide was transported under the Gulf Stream and remained isolated from the atmosphere for periods of decades or longer following the injection.
- *48 Students Enrolled in the Global Change Education Program for Undergraduate and Graduate Students* - Twenty-four outstanding undergraduate students were selected for participation in the 2001 DOE Summer Undergraduate Research Experience (SURE) and 24 exceptional graduate students were selected for DOE Graduate Research Environmental Fellowships (GREF), which provide support for their graduate research on climate change.

#### Environmental Remediation

- *Radiation Resistant Microbe Enzymatically Reduces Common Contaminants at DOE Sites* - The radiation resistant “superbug” *Deinococcus radiodurans* was shown by PNNL researchers to change chemical species of contaminants common to DOE sites (e.g., Uranium, Technetium, and Chromium) that are relatively soluble and mobile in water to insoluble and relatively immobile species. Under conditions where ionizing radiation is high, such as sediments and soils beneath leaking waste storage tanks at some DOE sites, *Deinococcus radiodurans* may provide a means for limiting the migration of multivalent radionuclides and heavy metals. Moreover, *Deinococcus* has now been reported to be endemic to the populations of soil microorganisms beneath radioactive waste storage tanks at the Hanford reservation, making this microbe especially promising for *in situ* bioremediation approaches.
- *Portable Immunoassay Instrument Developed for Quantitative Measurement of Uranium in the Field* - A field portable immunoassay has been developed to measure uranium, a common legacy waste contaminant at DOE sites. Researchers at Tulane University developed an immunosensor that can be used for speciation and quantification of uranium in groundwater. A prototype hand held instrument has been developed in collaboration with Sapidyne Instruments. This technology makes it possible to rapidly obtain information on levels of uranium contamination and the effectiveness of remediation approaches for reducing or stabilizing uranium contamination at DOE sites.

#### Medical Applications and Measurement Science

- *PET/Radiotracer Studies Help Anti-addiction Drug Development* - The Brookhaven National Laboratory (BNL) uses positron emission tomography (PET) and radiotracer techniques to study the brain mechanisms underlying addiction. PET and carbon-11 studies with Vigabatrin also known as GVG, a drug used to treat epilepsy outside the U.S., have shown that GVG may prove to be an effective pharmaceutical treatment for cocaine addiction. In subsequent studies, Brookhaven scientists and collaborators found that the drug effectively blocked test animals' craving for nicotine, heroin, alcohol, and methamphetamine.
- *Tracking the Brain Dopamine Pathology Related to Obesity* - PET and carbon -11 radiotracer drug studies at BNL, recently published in *Lancet* 357, 354-357, 2001, provide evidence of brain dopamine pathology in obesity. The studies have shown that the brains of obese people have abnormalities in the chemical dopamine that regulates pleasure centers in the brain.
- *New Radiotracers to Study Stroke* - Lawrence Berkley National Laboratory scientists have developed a new radiotracer probe to study the brain biochemistry relevant to stroke. The tritiated compound, known as drug candidate CNS5161, will be used first as a research tool in animal models of stroke, trauma, drug addiction, and memory consolidation. The carbon-11 labeled form of this compound will be developed to assess acute brain biochemical receptor activation in human stroke and head trauma as well as for monitoring the more chronic changes in neurodegenerative disorders.
- *Helping the Blind See* - A collaborative research project at The Johns Hopkins Wilmar Eye Institute and at Oak Ridge National Laboratory (ORNL) in Tennessee is developing a retinal prosthetic device (an artificial retina) that will allow patients who have retinitis pigmentosa or age-related macular degeneration to see again. Significant progress has been made on the development of a micro-imaging sensor that is small enough that it can be safely implanted into the eye. Preliminary results predict that patients with retinitis pigmentosa or age-related macular degeneration will have vision restored to a level equivalent to reading large print.
- *New Biological Microscope Wins Discover Award* - A new microscope, that pairs optical confocal microscopy with magnetic resonance microscopy, has been developed by scientists at the Environmental Molecular Sciences Laboratory (EMSL). This new microscope, which combines the unique features of both technologies, will allow researchers to visualize in living cells, important morphological changes that occur when normal healthy cells transform into tumor cells.
- *Polymer Formulations for Cartilage Repair* - Pacific Northwest National Laboratory (PNNL) researchers have demonstrated that temperature sensitive polymers can support cartilage-forming cell growth outside the body and also provide a temporary synthetic "scaffold" to support growth of the newly grown cartilage cells once they are injected back into the joint.
- *Mini-Camera for Fewer Biopsies in Breast Cancer Diagnosis* - Researchers at Hampton University and the Thomas Jefferson National Accelerator Facility developed a gamma mini-camera that uses a specially modified personal computer for data acquisition and analysis. The smaller camera coupled to a superior imaging and high-performance processing system provides better resolution of the breast and is expected to result in fewer biopsies.
- *New Method for Cancer Risk Assessment* - Scientists at Ames Laboratory have developed a chip-based, direct-readout methodology for detecting and quantifying DNA adducts, chemical compounds in which a carcinogen is attached to the DNA. These chemical compounds can be present long before cancer develops and are critical in understanding early events in carcinogenesis.

- *New Radiopharmaceuticals for Cancer Therapy* - Investigators at Duke University have developed iodine-131 and astatine-211 labeled antitenascin-antibody proteins for treatment of brain tumors such as gliomas. The antibody proteins carrying the therapeutic doses of radiation can selectively seek tenascin molecules located on glioma cancer cells, bind and deliver the radiation for effective cancer cell killing.

## FACILITY ACCOMPLISHMENTS

### Life Sciences

- *New Neutron User Facility for Structural Biologists* - DOE user facilities for structural biologists at the synchrotron light sources enable scientists to determine high resolution electron density maps of protein crystals needed to determine their three dimensional structure. In some cases, neutrons provide additional information critical to understand protein structure by providing vital insights into the locations of hydrogen bonds and the nature of macromolecular-solvent interactions. A new protein crystallography station at the Los Alamos Neutron Science Center (LANSCE) will be available by the end of 2002. This is the only neutron crystallography station for structural biologists in the U.S.
- *New Ultrasensitive Mass Spectrometer for Proteomics* - Pacific Northwest National Laboratory has developed a new electrospray ionization fourier transform ion cyclotron resonance mass spectrometer (ICR), the highest field and most sensitive ICR mass spectrometer currently available. This new machine is approximately 1000 fold more sensitive than conventional instruments, has a resolution 100-1000 fold greater than conventional instruments and can measure peptides at a level less than or equal to 1 part per million. At this level, most peptides are unique and can be assigned to a specific protein in the genome. In contrast, conventional instruments measure at approximately the 500 parts per million level.

### Environmental Remediation

- *Unique High Throughput Approach Using Mass Spectrometry for Proteome Characterization* - New mass spectrometry techniques developed by EMSL scientists are the basis for measuring changes in protein expression within a single experiment. This new approach can be used to monitor thousands to tens of thousands of proteins per day. The global perspective afforded by this new proteome measurement capability is diagnostic of changes within entire sets of cellular pathways and networks, thereby helps to identify those pathways key to a cell's state of development or response to a changing environment. The high throughput approach has been used to characterize the proteome of *Deinococcus radiodurans*, a microorganism with potential for bioremediating contaminated soils and groundwater. This approach confirmed almost half of the proteins predicted by genome annotation. Key to this successful project was the development of the ion funnel, a device that prevents ions in a sample from becoming lost by charge-charge repulsion of the ion beam as it is transferred into a mass spectrometer; greatly improved high pressure capillary liquid chromatographic separations; new methods for extending the dynamic range of measurements; and data processing methods that provide greater mass measurement accuracies for improved protein identification.

- *Computational and Experimental Chemistry Used to Determine New Estimate of Heat of Formation of OH Radical* - A team of scientists from EMSL and Argonne National Laboratory combined results from computational and experimental chemistry studies to determine a new value for the heat of formation of the hydroxyl radical (OH). This important result required use of the massively parallel supercomputer in EMSL and will have significant impact on models of combustion and atmospheric chemistry. The same approach has been used for many small, highly reactive species including those involved in fluorocarbon production and processing and the decomposition products of ammonia. Reliable prediction of the energetics of molecular systems is made possible by the revolution in computer hardware, software and computational methods and their application in computational chemistry.

## PROGRAM SHIFTS

For FY 2003, BER will focus on:

- Further developing the research infrastructure needed for Genomes to Life research. The development of virtual, distributed research centers, begun in FY 2002, will expand to include research capabilities needed for analyses of the functional capabilities of microbial populations comprised of multiple microbial species, enabling the development of strategies to use complex microbial communities to address DOE needs in clean energy production, carbon sequestration, and environmental cleanup.
- With the completion of the high quality DNA sequence of human chromosomes 5, 16, and 19, DNA sequencing capabilities at the Joint Genome Institute will increasingly emphasize the needs of research on microbes for energy, the environment, and national security and, through interagency partnerships, selected sequencing needs of other agencies including the National Science Foundation and the U.S. Department of Agriculture.
- In FY 2003 the Administration will launch a new Climate Change Research Initiative (CCRI). The CCRI will focus on research areas where substantial progress in both understanding and prediction are likely over the next five years, including climate variation and change, carbon cycle, water cycle, atmospheric composition, and regional impacts. BER will participate in one of the specific areas: understanding the North American Carbon Cycle.
- Bioremediation research will continue its focus on the biotransformation of radionuclides and metals at contaminated DOE sites, the community of microbes that affect the transformations in subsurface environments at the sites, and the development of strategies for using bioremediation to clean up or stabilize these contaminants at DOE sites.
- In FY 2003 the Environmental Management Science Program and the Savannah River Ecology Laboratory are transferred from the Office of Environmental Management (EM) to the Office of Science. BER will manage these research activities according to Office of Science principles, but with extensive input from EM.
- In FY 2003, funding for the followup of all patients treated in the human clinical trials of boron neutron capture therapy (BNCT) at Brookhaven National Laboratory and the Massachusetts Institute of Technology will be completed with the transfer of clinical technology to the National Cancer Institute of the National Institutes of Health. The basic drug development research program for BNCT will evolve into a new program of innovative approaches to cell-targeted ablation therapy for cancer with in-vivo radiation techniques. The emphasis of this program will be on the

therapeutic use of ionizing radiation that may be achieved with radionuclide therapy and novel methods of tumor targeting.

## **Genomes to Life Research**

The FY 2003 budget includes funds for the continued expansion of the research on microbes to address DOE's energy, environment, and national security mission needs. Initiated in FY 2002, this research will continue to more fully characterize the inventory of multiprotein molecular machines found in selected DOE-relevant microbes and higher organisms and to determine the functional diversity found in populations of microbes isolated from DOE-relevant sites. In FY 2003, new research will be initiated that focuses on further developing the research tools needed to study microbial communities that may have applications to clean energy, environmental cleanup, and carbon sequestration.

## **Climate Change Research Initiative**

In FY 2003, the Administration will institute a new Climate Change Research Initiative (CCRI). The CCRI is intended to focus research on areas where substantial progress in understanding and prediction are likely over the next five years, including climate variation and change, carbon cycle, water cycle, atmospheric composition, and regional impacts. The set of cross agency programs will have strong focus on outcomes and deliverables. DOE, in conjunction with other USGCRP agencies, will begin a focused research program in specific research areas. The deliverables will be targeted at information useful to policy-makers (e.g., provide quantitative estimates of the carbon balance in regions across the U.S.). DOE will participate in one of the specific research areas: understanding the North American Carbon Cycle (with NOAA, NSF, and USDA).

## **Scientific Facilities Utilization**

The Biological and Environmental Research request includes \$52,088,000 to maintain support of the Department's major scientific user facilities. Facilities include structural biology research beam lines at the synchrotron light sources and the operation of the William R. Wiley Environmental Molecular Sciences Laboratory where research activities underpin long-term environmental remediation and other DOE missions in energy and national security. With this funding, BER will provide for the operation of the facilities, assuring access for scientists in universities, federal laboratories, and industry. BER will also leverage both federally and privately sponsored research.

## **Workforce Development**

Workforce development is an integral and essential element of the BER mission to help ensure a science-trained workforce, including researchers, engineers, science educators, and technicians. The research programs and projects at the National Laboratories, universities, and research institutes actively integrate undergraduate and graduate students and post-doctoral investigators into the work. This "hands-on" approach is essential for the development of the next generation of scientists, engineers, and science educators. Specific fellowship programs are also sponsored by BER to target emerging areas of need. Over 1,500 graduate students and post-doctoral investigators will be supported at universities and at National Laboratories in FY 2002. BER will continue its support for graduate students and post-doctoral investigators in FY 2003. The number of graduate students and post-doctoral investigators will remain approximately at the FY 2002 level.

Graduate students and postdoctoral investigators use Office of Science user facilities. For example, they use the structural biology experimental stations on the beam lines at the synchrotron light sources and the instruments at the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL). Using

these unique research tools enables the graduate students and post-doctoral investigators to participate in and conduct leading edge research. Approximately half of all of the facility users are graduate students and postdoctoral investigators. The graduate students and post doctoral investigators are supported by resources from a wide variety of sponsors, including BER, other Departmental research programs, other federal agencies, and U.S. and international private institutions. Graduate students and post-doctoral investigators at the synchrotron light sources are included in the Basic Energy Sciences (BES) user facility statistics and are not included here. A total of 500 graduate students and post-doctoral investigators conducted their research at the EMSL in FY 2001.

BER will continue its commitment to and dependence on research scientists at the Nation's universities. Approximately 40 percent of BER basic research funding directly supports university-based activities. University scientists are the major users at BER facilities and other enabling research infrastructure. University-based scientists are an integral part of research programs across the entire range of the BER portfolio. These scientists are funded through individual peer-reviewed grants and as members of peer-reviewed research teams involving both national laboratory and university scientists.

University-based scientists are the principal users of BER user facilities for structural biology at the synchrotron and neutron sources. They are also users of the Environmental Molecular Sciences Laboratory, and the Natural and Accelerated Bioremediation Research (NABIR) program's Field Research Center. University scientists also form the core of the Atmospheric Radiation Measurement (ARM) science team that networks with the broader academic community as well as with scientists at other agencies, such as the National Aeronautics and Space Administration and the National Oceanic and Atmospheric Administration. In addition, university-based scientists are funded through Requests for Applications across the entire BER program including genomics, structural biology, low dose radiation research, global change research, bioremediation research, medical imaging, and radiopharmaceutical development. Furthermore, university scientists work in close partnership with scientists at National Laboratories in many BER programs including genomics, and carbon sequestration research.



## Funding Profile

(dollars in thousands)

	FY 2001 Comparable Appropriation	FY 2002 Original Appropriation	FY 2002 Adjustments	FY 2002 Comparable Current Appropriation	FY 2003 Request
Biological and Environmental Research					
Life Sciences .....	188,469	193,385	-812	192,573	210,878
Climate Change Research ....	125,678	129,469	-547	128,922	137,959
Environmental Remediation ..	104,235	69,637	+44,764	114,401	109,530
Medical Applications and Measurement Science.....	93,187	123,509	-510	122,999	45,848
Subtotal, Biological and Environmental Research.....	511,569	516,000	+42,895	558,895	504,215
Construction .....	2,495	11,405	--	11,405	0
Subtotal, Biological and Environmental Research.....	514,064	527,405	+42,895	570,300	504,215
General Reduction.....	--	-2,155	2,155	0	--
Total, Biological and Environmental Research.....	514,064 <sup>a b c</sup>	525,250	45,050	570,300 <sup>c</sup>	504,215

### Public Law Authorization:

Public Law 95-91, "Department of Energy Organization Act"

Public Law 103-62, "Government Performance and Results Act of 1993"

<sup>a</sup> Excludes \$11,088,000 which was transferred to the SBIR program and \$665,000 which was transferred to the STTR program.

<sup>b</sup> Excludes \$650,000 which was transferred to the Science Safeguards and Security program in an FY 2001 reprogramming.

<sup>c</sup> Includes \$43,947,000 in FY 2001 and \$45,050,000 in FY 2002 for Environmental Management Science Program and Savannah River Ecology Laboratory being transferred from Environmental Management.

## Funding By Site

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
<b>Albuquerque Operations Office</b>					
Los Alamos National Laboratory.....	22,447	19,848	18,681	-1,167	-5.9%
Sandia National Laboratories .....	3,474	3,391	2,737	-654	-19.3%
Albuquerque Operations Office .....	1,597	900	850	-50	-5.6%
<b>Total, Albuquerque Operations Office .....</b>	<b>27,518</b>	<b>24,139</b>	<b>22,268</b>	<b>-1,871</b>	<b>-7.8%</b>
<b>Chicago Operations Office</b>					
Ames Laboratory .....	1,066	690	512	-178	-25.8%
Argonne National Laboratory – East .....	27,521	23,067	22,595	-472	-2.0%
Brookhaven National Laboratory .....	23,549	18,862	15,993	-2,869	-15.2%
Chicago Operations Office.....	92,092	47,702	46,146	-1,556	-3.3%
<b>Total, Chicago Operations Office .....</b>	<b>144,228</b>	<b>90,321</b>	<b>85,246</b>	<b>-5,075</b>	<b>-5.6%</b>
<b>Idaho Operations Office</b>					
Idaho National Engineering & Environmental Laboratory.....	1,440	1,056	400	-656	-62.1%
Idaho Operations Office.....	37,029	37,050	29,886	-7,164	-19.3%
<b>Total, Idaho Operations Office .....</b>	<b>38,469</b>	<b>38,106</b>	<b>30,286</b>	<b>-7,820</b>	<b>-20.5%</b>
<b>Oakland Operations Office</b>					
Lawrence Berkeley National Laboratory.....	61,970	50,133	44,821	-5,312	-10.6%
Lawrence Livermore National Laboratory.....	33,450	32,715	36,899	+4,184	+12.8%
Stanford Linear Accelerator Center .....	3,656	4,170	5,550	+1,380	+33.1%
Oakland Operations Office .....	70,815	46,043	38,386	-7,657	-16.6%
<b>Total, Oakland Operations Office .....</b>	<b>169,891</b>	<b>133,061</b>	<b>125,656</b>	<b>-7,405</b>	<b>-5.6%</b>
<b>Oak Ridge Operations Office</b>					
Oak Ridge Inst. For Science & Education .....	5,179	4,893	4,761	-132	-2.7%
Oak Ridge National Laboratory .....	45,798	45,134	33,085	-12,049	-26.7%
Oak Ridge Operations Office.....	380	352	352	0	--
Thomas Jefferson National Accelerator Facility ...	620	400	500	+100	+25.0%
<b>Total, Oak Ridge Operations Office .....</b>	<b>51,977</b>	<b>50,779</b>	<b>38,698</b>	<b>-12,081</b>	<b>-23.8%</b>

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
Richland Operations Office					
Pacific Northwest National Laboratory .....	72,618	73,383	73,052	-331	-0.5%
Savannah River Operations Office .....	7,880	8,000	5,841	-2,159	-27.0%
Washington Headquarters .....	1,483	152,511	123,168	-29,343	-19.2%
Total, Biological and Environmental Research.....	514,064 <sup>a b c</sup>	570,300 <sup>c</sup>	504,215	-66,085	-11.6%

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<sup>a</sup> Excludes \$11,088,000 which was transferred to the SBIR program and \$665,000 which was transferred to the STTR program.

<sup>b</sup> Excludes \$650,000 which was transferred to the Science Safeguards and Security program in an FY 2001 reprogramming.

<sup>c</sup> Includes \$43,947,000 in FY 2001 and \$45,050,000 in FY 2002 for Environmental Management Science Program and Savannah River Ecology Laboratory being transferred from Environmental Management.

## **Site Description**

### **Ames Laboratory**

Ames Laboratory is a Multiprogram Laboratory located on 10 acres in Ames, Iowa. At Ames, BER supports research into new biological imaging techniques such as the study of gene expression in real time and fluorescence spectroscopy to study environmental carcinogens.

### **Argonne National Laboratory**

Argonne National Laboratory (ANL) in Argonne, Illinois, is a Multiprogram Laboratory located on a 1,700 acre site in suburban Chicago. ANL has a satellite site located in Idaho Falls, Idaho. At ANL, BER supports the operation of a high-throughput national user facility for protein crystallography at the Advanced Photon Source. In support of climate change research, ANL coordinates the operation and development of the Southern Great Plains, Tropical Western Pacific, and North Slope of Alaska ARM sites. The principal scientist for the Atmospheric Chemistry program is at ANL, providing broad scientific integration to the program. Research is conducted to understand the molecular control of genes and gene pathways in microbes. ANL, in conjunction with ORNL and PNNL and six universities, co-hosts the terrestrial carbon sequestration research center, CSiTE.

### **Brookhaven National Laboratory**

Brookhaven National Laboratory (BNL) is a Multiprogram Laboratory located on a 5,200 acre site in Upton, New York. BER supports the operation of beam lines for protein crystallography at the National Synchrotron Light Source for use by the national biological research community, research in biological structural determination, and research into new instrumentation for detecting x-rays and neutrons. Research is also conducted on the molecular mechanisms of cell responses to low doses of radiation.

The radiotracer chemistry, radiopharmaceutical technology, and magnetic resonance imaging research and development programs support applications of novel techniques for imaging brain function in normal and diseased states, and to study the biochemical basis of disease.

Global change activities at BNL include the operation of the ARM External Data resource that provides ARM investigators with data from non-ARM sources, including satellite and ground-based systems. BNL scientists form an important part of the science team in the Atmospheric Sciences program, providing special expertise in atmospheric field campaigns and aerosol research. BNL scientists play a leadership role in the development of, and experimentation at, the Free-Air Carbon Dioxide Enhancement (FACE) facility at the Duke Forest used to understand how plants respond to elevated carbon dioxide concentrations in the atmosphere.

## **Idaho National Engineering and Environmental Laboratory**

Idaho National Engineering and Environmental Laboratory (INEEL) is a Multiprogram Laboratory located on 572,000 acres in Idaho Falls, Idaho. Using unique DOE capabilities such as advanced software for controlling neutron beams and calculating dose, BER supports research into boron chemistry, radiation dosimetry, analytical chemistry of boron in tissues, and engineering of new systems for application of this treatment technique to tumors, including brain tumors. Research is also supported into the analytical chemistry of complex environmental and biological systems using the technique of mass spectrometry.

## **Lawrence Berkeley National Laboratory**

Lawrence Berkeley National Laboratory (LBNL) is a Multiprogram Laboratory located in Berkeley, California. The Laboratory is on a 200 acre site adjacent to the Berkeley campus of the University of California. LBNL is one of the major national laboratory partners that comprise the Joint Genome Institute (JGI) whose principal goals are high-throughput DNA sequencing techniques and studies on the biological functions associated with newly sequenced human DNA. A significant component of the JGI's sequencing goal is the development and integration of instrumentation, automation, biological resources, and data management and analysis tools into a state-of-the-art DNA sequencing assembly line that is highly efficient and cost effective. The laboratory also conducts research on the molecular mechanisms of cell responses to low doses of radiation and on the use of model organisms to understand and characterize the human genome.

LBNL operates beam lines for determination of protein structure at the Advanced Light Source for use by the national biological research community, research into new detectors for x-rays, and research into the structure of proteins, including membrane proteins.

The nuclear medicine program supports research into novel radiopharmaceuticals for medical research and studies of novel instrumentation for imaging of living systems for medical diagnosis.

LBNL supports the Natural and Accelerated Bioremediation Research (NABIR) program and the geophysical and biophysical research capabilities for NABIR field sites. BER supports research at LBNL into new technologies for the detailed characterization of complex environmental contamination. LBNL also develops scalable implementation technologies that allow widely used climate models to run effectively and efficiently on massively parallel processing supercomputers. The carbon cycle field experiment at the ARM Southern Great Plains site is maintained and operated by LBNL.

## **Lawrence Livermore National Laboratory**

Lawrence Livermore National Laboratory (LLNL) is a Multiprogram Laboratory located on an 821 acre site in Livermore, California. LLNL is one of the major national laboratory partners that comprise the Joint Genome Institute (JGI) whose principal goals are high-throughput DNA sequencing and studies on the biological functions associated with newly sequenced human DNA. A significant component of the JGI's sequencing goal, is the development and integration of instrumentation, automation, biological resources, and data management and analysis tools into a state-of-the-art DNA sequencing assembly line that is highly efficient and cost effective. LLNL also conducts research on the molecular mechanisms of cell responses to low doses of radiation, and on the use of model organisms to understand and characterize the human genome.

Through the program for Climate Model Diagnostics and Intercomparison, LLNL provides the international leadership to understand and improve climate models. Virtually every climate modeling center in the world participates in this unique program.

### **Los Alamos National Laboratory**

Los Alamos National Laboratory (LANL) is a Multiprogram Laboratory located on a 27,000 acre site in Los Alamos, New Mexico. LANL is one of the major national laboratory partners that comprise the Joint Genome Institute (JGI) whose principal goals are high-throughput DNA sequencing and studies on the biological functions associated with newly sequenced human DNA. A significant component of the JGI's sequencing goal is the development and integration of instrumentation, automation, biological resources, and data management and analysis tools into a state-of-the-art DNA sequencing assembly line that is highly efficient and cost effective. One of LANL's roles in the JGI involves the production of high quality "finished" DNA sequence. LANL also conducts research on the molecular mechanisms of cell responses to low doses of radiation and on research to understand the molecular control of genes and gene pathways in microbes. Activities in structural biology include the operation of an experimental station for protein crystallography at the Los Alamos Neutron Science Center for use by the national biological research community and research into new techniques for determination of the structure of proteins.

LANL provides the site manager for the Tropical Western Pacific ARM site. LANL also has a crucial role in the development, optimization, and validation of coupled atmospheric and oceanic general circulation models using massively parallel computers.

LANL also conducts research into advanced medical imaging technologies for studying brain function and research into new techniques for rapid characterization and sorting of mixtures of cells and cell fragments.

### **Oak Ridge Institute for Science and Education**

Oak Ridge Institute for Science and Education (ORISE) is located on a 150 acre site in Oak Ridge, Tennessee. ORISE coordinates several research fellowship programs for BER. ORISE also coordinates activities associated with the peer review of most of the research proposals submitted to BER.

ORISE conducts research into modeling radiation dosages for novel clinical diagnostic and therapeutic procedures.

### **Oak Ridge National Laboratory**

Oak Ridge National Laboratory (ORNL) is a Multiprogram Laboratory located on a 24,000 acre site in Oak Ridge, Tennessee. ORNL has a leadership role in research focused on the ecological aspects of global environmental change. The Throughput Displacement Experiment at the Walker Branch Watershed is a unique resource for long term ecological experiments. ORNL is the home of the newest FACE experiment supported by BER. ORNL also houses the ARM archive, providing data to ARM scientists and to the general scientific community. ORNL scientists provide improvement in formulations and numerical methods necessary to improve climate models. ORNL scientists make important contributions to the NABIR program, providing special leadership in microbiology applied in

the field. ORNL also manages the NABIR Field Research Center, a field site for developing and testing bioremediation approaches to remediate metal and radionuclide contaminants in subsurface environments.

ORNL conducts research on widely used data analysis tools and information resources that can be automated to provide information on the biological function of newly discovered genes identified in high-throughput DNA sequencing projects. The laboratory also uses mice as model organisms to understand and characterize the human genome.

ORNL conducts research into the application of radioactively labeled monoclonal antibodies in medical diagnosis and therapy, particularly of cancer, as well as research into new instrumentation for the analytical chemistry of complex environmental contamination using new types of biosensors.

ORNL recently has upgraded the High Flux Isotope Reactor (HFIR) to include a cold neutron source that will have high impact on the field of structural biology. BER is developing a station for Small Angle Neutron Scattering at HFIR to serve the structural biology community.

ORNL, in conjunction with ANL and PNNL and six universities, co-hosts a terrestrial carbon sequestration research center, CSiTE.

## **Pacific Northwest National Laboratory**

Pacific Northwest National Laboratory (PNNL) is a Multiprogram Laboratory located on 640 acres at the Department's Hanford site in Richland, Washington. PNNL is home to the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL). PNNL scientists, including EMSL scientists, play important roles in both supporting the NABIR program and in performing research for NABIR.

PNNL operates the unique ultrahigh field mass spectrometry and nuclear magnetic resonance spectrometry instruments at the Environmental Molecular Sciences Laboratory for use by the national biological research community.

PNNL provides the lead scientist for the Environmental Meteorology Program, the G-1 research aircraft, and expertise in field campaigns. PNNL provides the planning and interface for the Climate Change Prediction Program with other climate modeling programs. The ARM program office is located at PNNL, as is the ARM chief scientist and the project manager for the ARM engineering activity; this provides invaluable logistical, technical, and scientific expertise for the program.

PNNL conducts research into new instrumentation for microscopic imaging of biological systems and for characterization of complex radioactive contaminants by highly automated instruments.

PNNL conducts research on the molecular mechanisms of cell responses to low doses of radiation and on the development of high throughput approaches for characterizing all of the proteins (the proteome) being expressed by cells under specific environmental conditions.

PNNL, in conjunction with ANL and ORNL and six universities, co-hosts a terrestrial carbon sequestration research center, CSiTE.

PNNL also conducts research on the integrated assessment of global climate change.

In March 2001 the University of Maryland and Pacific Northwest National Laboratory created a Joint Global Change Research Institute in College Park, Maryland. The Institute investigates the scientific, social, and economic implications of climate change, both nationally and globally. BER funding

supports research grants to the university and research projects to PNNL that have been successfully peer reviewed in open competition.

### **Sandia National Laboratory**

Sandia National Laboratory (SNL) is a Multiprogram Laboratory, with a total of 3,700 acres, located in Albuquerque, New Mexico, with sites in Livermore, California and Tonopah, Nevada. SNL provides the site manager for the North Slope of Alaska ARM site. The chief scientist for the ARM-UAV program is at SNL, and SNL takes the lead role in coordinating and executing ARM-UAV missions. The laboratory conducts advanced research and technology development in robotics, smart medical instruments, microelectronic fabrication, and computational modeling of biological systems.

To support environmental cleanup, SNL conducts research into novel sensors for analytical chemistry of contaminated environments.

### **Savannah River Site**

The Savannah River Site complex covers 198,344 acres, or 310 square miles encompassing parts of Aiken, Barnwell and Allendale counties in South Carolina bordering the Savannah River. At the Savannah River Site, BER supports the Savannah River Ecology Laboratory (SREL), a research unit of the University of Georgia operating at the site for over forty years. The SREL conducts research aimed at reducing the cost of environmental cleanup and remediation while ensuring biodiversity to the restored environment.

BER supports the Savannah River Ecology Laboratory through a cooperative agreement with the University of Georgia. The ecological research activity is aimed at reducing the cost of cleanup and remediation while ensuring biodiversity to the restored environment.

### **Stanford Linear Accelerator Center**

Stanford Linear Accelerator Center (SLAC) is a program-dedicated laboratory (High Energy Physics) located on 426 acres in Menlo Park, California, and is the home of the Stanford Synchrotron Radiation Laboratory (SSRL). The Stanford Synchrotron Radiation Laboratory was built in 1974 to utilize the intense x-ray beams from the SPEAR storage ring that was built for particle physics by the SLAC laboratory. Over the years, the SSRL grew to be one of the main innovators in the production and use of synchrotron radiation with the development of wigglers and undulators that form the basis of all third generation synchrotron sources. The facility is now comprised of 25 experimental stations and is used each year by over 700 researchers from industry, government laboratories and universities. Through the Stanford Linear Accelerator Center, BER (in coordination with the National Institutes of Health) is funding the operation of nine Stanford Synchrotron Radiation Laboratory beam lines for structural biology. This program involves synchrotron radiation-based research and technology developments in structural molecular biology that focus on protein crystallography, x-ray small angle scattering diffraction, and x-ray absorption spectroscopy for determining the structures of complex proteins of many biological consequences.



## **Thomas Jefferson National Accelerator Facility**

The Thomas Jefferson National Accelerator Facility (TJNAF) is a basic research laboratory located on a 200 acre site in Newport News, Virginia. BER supports the development of advanced imaging instrumentation at TJNAF that will ultimately be used in the next generation medical imaging systems.

## **All Other Sites**

The BER program funds research at nearly 340 institutions, including colleges/universities, private industry, and other federal and private research institutions located in 43 states. Also included are funds for research awaiting distribution pending completion of peer review procedures.

BER supports a broad range of peer-reviewed research at America's universities, including institutions that traditionally serve minority communities. BER research opportunities are announced through public solicitations in the Federal Register for research applications from universities and the private sector.

BER's Life Sciences research is conducted at a large number of universities in all aspects of the program. Research is conducted in support of high-throughput human DNA sequencing at the JGI, on the sequencing of entire microbial genomes with value to the DOE mission, to understand the molecular control of genes and gene pathways in microbes, on the use of model organisms to understand and characterize the human genome, and on the molecular mechanisms of cell responses to low doses of radiation.

In structural biology, universities provide new imaging detectors for x-rays, research in computational structural biology directed at the understanding of protein folding, and research into new techniques such as x-ray microscopy.

Peer-reviewed projects are supported in each element of the Climate Change Research subprogram, with very active science teams, in particular, in the Atmospheric Chemistry Program and the ARM programs. Academic investigators are essential to the Integrated Assessment portfolio.

In the NABIR program, academic and private sector investigators are performing research in areas that include mechanistic studies of bioremediation of actinide and transition metal contamination, the structure of microbial communities in the presence of uranium and other such contaminants, gene function in microorganisms with degradative properties, geochemical and enzymatic processes in microbial reduction of metals, and the use of tracers to monitor and predict metabolic degradative activity.

In the nuclear medicine program, universities conduct research into new types of radiopharmaceuticals, particularly those based on application of concepts from genomics and structural biology. BER places emphasis on radiopharmaceuticals that will be of use in advanced imaging techniques such as positron emission tomography. The research supports new instrumentation for medical imaging. The BER Measurement Science program supports research into novel types of biosensors for medical imaging and application in analytical chemistry of contaminated environments.

# Life Sciences

## Mission Supporting Goals and Objectives

The goal of the Life Sciences subprogram is to deliver knowledge in structural biology, genomics, and the health effects of low dose radiation. Human, animal, and microbial DNA sequencing will be used to understand the genetic and environmental basis of normal and abnormal function. Scientific tools will be developed to understand gene function and protein structure needed for biotechnology solutions for clean energy, carbon sequestration, environmental cleanup, and bioterrorism detection and defeat. Low dose radiation research will provide knowledge for rigorous, cost-effective standards to protect the health of cleanup workers and the public and for science-based decisions on DOE site cleanup operations.

BER's Life Sciences research is focused on developing, making available, and using unique DOE resources and facilities to understand and mitigate potential health effects of energy development, energy use, and waste cleanup, and develop novel biotechnology solutions for energy, environmental, and national security applications. BER supports research in five areas: structural and computational biology, low dose radiation, microbial biology, human genome, and biological research.

- BER develops and supports user facilities for the Nation's structural biologists; combines computer science, structural biology, and genome research for analyses and predictions of gene function from the individual gene to the genomic level; and develops new technologies and methodologies to understand the dynamic processes of protein-protein interactions that are unique to living organisms.
- BER supports research on low dose and low dose-rate radiation and addresses both the scientific issues and results with scientists, regulators, and the public to provide a better scientific basis for achieving acceptable levels of human health protection from low levels of ionizing radiation.
- BER takes advantage of the remarkable diversity of microbes found in the environment and our ability to identify and to understand how biological functions follow from the DNA sequence to the behavior of an entire organism. This information can help in the development of unique solutions in energy production, waste cleanup, and carbon management.
- BER is an integral part of the International Human Genome Project that has made publicly available a highly accurate sequence of the human DNA sequence. The BER Human Genome program also develops resources, tools, and technologies needed to analyze and interpret DNA sequence data from entire organisms, determines the function of the genes identified from DNA sequencing, and studies the ethical, legal, and social implications (ELSI) of information and data resulting from the genome project.
- Finally, BER's research program is developing the capability to predict how single cells and multi-cellular organisms respond to biological and environmental cues and to use this predictive capability to address DOE needs in energy, the environment, and for national security. This challenge starts with the remarkable progress being made in all other parts of the Life Sciences subprogram, from DNA sequencing to structural biology, and requires the development of new technologies, analytical methods, and modeling capabilities.

The Life Sciences subprogram's support of microbial genome research also contributes to the BER clean energy and carbon sequestration research programs. Knowing the genomic sequence of microbes that are involved in carbon sequestration or that produce methane and hydrogen, is enabling the identification of the key genetic and protein components of the organisms that regulate these processes. Understanding more fully how the enzymes and organisms operate will enable scientists to evaluate their potential use to remove excess carbon dioxide from the atmosphere or to produce methane or hydrogen from either fossil fuels or other carbonaceous sources, including biomass or even some waste products. Recently discovered extremophile organisms could be used to engineer biological entities that could ingest a feedstock like methane, produce hydrogen, and sequester the carbon dioxide by-product.

### Funding Schedule

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
Structural Biology .....	35,975	27,927	27,847	-80	-0.3%
Molecular and Cellular Biology .....	49,387	58,272	73,264	+14,992	+25.7%
Human Genome.....	85,491	87,858	90,185	+2,327	+2.6%
Health Effects.....	17,616	13,640	14,251	+611	+4.5%
SBIR/STTR .....	0	4,876	5,331	+455	+9.3%
<b>Total, Life Sciences .....</b>	<b>188,469</b>	<b>192,573</b>	<b>210,878</b>	<b>+18,305</b>	<b>+9.5%</b>

### Detailed Program Justification

(dollars in thousands)

	FY 2001	FY 2002	FY 2003
<b>Structural Biology</b>	<b>35,975</b>	<b>27,927</b>	<b>27,847</b>
■ <b>Basic Research</b> .....	<b>12,012</b>	<b>12,627</b>	<b>12,547</b>

BER will continue to invest in structural biology research. In biology, most proteins do not act independently in living systems. In carrying out their functions within cells, proteins form complexes with other proteins (molecular machines) and interact with a variety of structural and regulatory molecules on which proteins carry out their functions. The role of structure in determining protein interactions with diverse molecules in a cell is still poorly understood. Understanding how molecular machines carry out their biological functions requires that we observe dynamic changes in protein structure and study protein modifications, translocation, and subcellular concentrations.

Starting with DNA sequencing information, research is supported to predict or identify the proteins that are involved in the recognition or repair of radiation-induced DNA damage or in the bioremediation of metals and radionuclides that could lead to reduced clean up costs; and to determine the high-resolution three-dimensional structures of those proteins. To fully understand

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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the mechanisms underlying the behavior of the molecular machines that carry out these functions, research is conducted and computer simulation models are developed: (1) on the dynamic changes in protein structure associated with protein modification and with protein-protein and protein-nucleic acid interactions that occur in these molecular machines; (2) to develop instrumentation that enables imagery of molecular machines in real-time at high levels of resolution; and (3) to precisely measure their intracellular compartmentalization and translocations.

DOE investment in structural biology research is having a large impact on basic research investments being made by other agencies. DOE investments in structural biology user facilities at synchrotron light sources and at the Environmental Molecular Sciences Laboratory (EMSL) and in development of key technologies for speeding the determination of protein structure have enabled the National Institute of General Medical Sciences at the National Institutes of Health (NIH) to make a large investment (over \$25,000,000 per year from FY 2001 to FY 2005) in pilot projects for NIH's Protein Structure Initiative to develop high throughput methods for determining protein structure. Six of the seven initial pilot projects, funded by NIH, include partners from DOE Laboratories and nearly all are centered around DOE user facilities.

**Performance will be measured** by the development of experimental and computational models that can successfully predict which proteins interact with protein complexes involved in DNA damage recognition and repair or bioremediation of metals and radionuclides from analysis of DNA sequence.

- **Infrastructure Development** ..... **23,963**    **15,300**    **15,300**

BER supports and develops beamlines and instrumentation for the Nation's structural biologists. It coordinates with the NIH and the NSF development and operation of experimental stations at DOE synchrotrons (Advanced Photon Source, Advanced Light Source, Stanford Synchrotron Radiation Laboratory and National Synchrotron Light Source) and neutron beam sources (the Los Alamos Neutron Science Center (LANSCE) and High Flux Isotope Reactor at ORNL). BER also supports access to mass spectrometry and nuclear magnetic resonance spectrometry user facilities at the EMSL that are used for both proteomic and structural biology research. University scientists are the principal users of these facilities.

**Performance will be measured** by having more than 2,500 highly satisfied users of the structural biology instruments at the DOE national user facilities.

By the end of FY 2003, BER's new (funded in FY 2001) DNA Repair Protein Complex Beamline at the Advanced Light Source at Lawrence Berkeley National Laboratory will be operational and available for users. This beamline will have novel features that include the ability to conduct both high-resolution (2 Angstrom) and low-resolution (2000 Angstrom) studies on important biomolecules using the same beamline. It will meet a rapidly growing need in the structural biology user community to provide unique information on functionally important conformational changes of multiprotein complexes and on factors that regulate the assembly of those complexes.

(dollars in thousands)

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BER also operates the neutron protein crystallography station at the Los Alamos Neutron Science Center (LANSCE) and will complete a new station for small angle neutron scattering at the High Flux Isotope Reactor (HFIR) at ORNL.

**Performance will be measured** by having ten external user groups use the LANSCE protein crystallography station and by beginning the commissioning of the Biological Small Angle Neutron Scattering Station at the Oak Ridge National Laboratory High Flux Isotope Reactor by the end of FY 2003.

BER also supports, with NSF and NIH, the Protein Data Bank for three-dimensional protein structures, a resource of growing importance that serves the NIH's high throughput structural genomics initiative as well as the Nation's life sciences research programs.

Unique facilities being developed at BER's Environmental Molecular Sciences Laboratory (EMSL) are now being made available to the structural biology user community.

**Performance will be measured** by the number of users resulting from the use of advanced mass spectrometry and nuclear magnetic resonance instrumentation at the Environmental Molecular Sciences Laboratory (EMSL) for structural biology and proteomics research.

<b>Molecular and Cellular Biology</b> .....	<b>49,387</b>	<b>58,272</b>	<b>73,264</b>
■ <b>Microbial Genomics</b> .....	<b>13,345</b>	<b>10,868</b>	<b>10,928</b>
■ <i>Microbial genomics research addresses DOE mission needs</i> – The program continues to sequence microbes that will be used to impact several DOE missions including: microbes for energy production (methane or hydrogen producing microbes), as alternative fuel sources (methane production or energy from biomass), for carbon sequestration, for helping to clean up the environment, and that are related to potential biothreat agents. The underlying scientific justification remains a central principle of the BER genome programs – complete genomic sequences yield answers to fundamental questions in biology. Knowing the complete DNA sequence of a microbe provides important keys to the biological capabilities of that organism and is the first step in developing strategies to more efficiently detect, counteract, use, or reengineer that microbe to address DOE needs.			
■ <i>Scientific needs of the DOE microbial genome program</i> – Now that the DNA sequence of more than 50 microbes with potential uses in energy, waste cleanup, and carbon sequestration have been determined, the program is beginning to further interpret and use that DNA sequence information. In FY 2003, the microbial genome program will continue to focus on 5 scientific challenges:			
■ <i>Functional analysis</i> - It is presently difficult to predict biological function of novel genes from genomic sequence data. The program is developing better experimental and computational methods to identify these novel genes and predict the functions of the proteins they encode.			

(dollars in thousands)

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- *Bioinformatics* – More than a third of the nearly 100 publicly available genomic sequences of archaea and bacteria are a result of DOE Microbial Genome program funding. Novel computational tools are being developed to increase the value of microbial genomic information, such as identifying distant relationships of genes, understanding microbial evolution, predicting gene function, identifying and modeling gene expression networks, and extracting longer stretches of useable DNA sequence from raw sequence data.
- *Microbial Genomic Plasticity* – Current microbial DNA sequence data strongly suggests that entire blocks of genes have been transferred between microbes during evolution. Research is being conducted to assess the frequency, mechanisms, and circumstances of lateral gene exchanges among microbes. This understanding is important for interpreting sequence data and for designing novel strategies for using microbes to address DOE mission needs.
- *Novel Approaches to Microbial Genomic Sequencing* - Research is being conducted on new methods to accelerate sequence comparisons without resequencing the entire genome of the related organism from scratch. Emphasis is being placed on novel uses of proven technologies with a particular emphasis on the identification of specific DNA sequence features that are associated with phenotypic differences between the microbes being compared.
- *Consortia and Hard-to-Culture Microbes* – Most microbes in the environment neither live in isolation from other microbes or can be readily grown in the laboratory. Research is focused on the organization, membership, or functioning of consortia of microbes, especially those involved in environmental processes of interest to DOE or that use potential biothreat agents, and on the development of technologies that enable genomic analyses of these consortia without the need for isolating individual microbes.

**Performance will be measured** by drafting genomic sequence of more than 30 microorganisms of high DOE relevance and scientific research; improving the computational tools for predicting gene function; and by the development of methods for sequencing unculturable microbes and microbial consortia.

- **Carbon Sequestration Research** ..... **7,127**      **7,107**      **7,138**  
 Microbes play a substantial role in the global cycling of carbon through the environment. The main emphasis of the program in FY 2003 is to leverage this new genomic DNA sequence information to characterize key biochemical pathways or genetic regulatory networks in these microbes. Analysis of biochemical pathways has previously focused on single genes or small numbers of genes at one time. Research in this program will focus, as described above, on the development and use of new, high-throughput technologies to determine the function of new genes discovered from microbial DNA sequencing. The information on the DNA sequence, key reaction pathways, and genetic regulatory networks will be used to develop strategies to use microbes and other organisms capable of carbon sequestration more efficiently or to even reengineer these organisms to enhance their capacity to sequester excess atmospheric carbon.

(dollars in thousands)

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**Performance will be measured** by the completion of a draft 3x DNA sequence of a member of the genus *Populus* (trees like poplar, aspen, etc.). These rapidly growing trees not only offer an opportunity for carbon sequestration, but also for bioremediation and energy from biomass. In addition, *Thalassiosira*, a diatom important in oceanic sequestration will also be draft sequenced.

■ **Genomes to Life** ..... **9,361**    **21,514**    **36,675**

Research on microbes that address DOE energy, environmental, and national security needs continues to expand in FY 2003 as a research program on the leading edge of biology. The research will offer new biotechnology solutions to challenges related to DOE’s missions in, for example, new clean energy sources, climate stabilization through carbon sequestration, toxic waste cleanup, and biothreat reduction.

Microbes and plants are responsible for the initial production of essentially all carbon-based energy that we use, whether from oil, coal or biomass, and for the subsequent removal of the energy-related carbon from the atmosphere. Microbes and microbial communities also make up about 60% of the biomass on Earth and have the potential to make a substantial impact on energy production, sequestration of carbon from the atmosphere, and the cleanup of hazardous waste. A deeper, genetically based understanding of these organisms, culminating in computational models of their function that can be used to predict and even modify their functions or efficiencies, promises a revolution in energy production, use, and environmental impact. This research program is part of an interagency program to understand life’s basic processes to meet National goals in many areas including health, agriculture, and energy.

The availability of complete genome sequences for all manner of life on Earth has opened a new era and new opportunities in biology. Research on the biological processes involved in the carbon cycle will lead to new biological strategies for storing and monitoring carbon. Understanding metabolic pathways and their regulatory networks will allow us to more effectively use or create designer microbes or plants that produce and convert biomass for fuel, power, and products. Harnessing metabolic or regulatory pathways in hydrogen-producing microbes could provide an alternative and ultimately clean energy source. This new understanding will also enable development of better detection and prevention strategies for potential biothreat agents.

We are just beginning to appreciate the potential applications of microorganisms. For all intents and purposes, ours is a microbial world filled with microscopic creatures that we take for granted and almost never even know are there. Microorganisms are Earth’s recyclers, participating in the recycling of most biological materials on Earth. In the process they produce and, together with plants, take up greenhouse gases. Microbes in particular have evolved on Earth for some 3.8 billion years and, as suggested by their diversity and range of adaptation, have long ago solved many problems for which DOE is seeking solutions. It has been estimated that more than 99% of Earth’s genetic and metabolic diversity, and, importantly, Earth’s useable potential, reside in the microbial universe of bacteria, fungi, archaea, and minute protozoa and micro algae that collectively comprise the planktonic communities in the oceans and the majority of life in soil.

(dollars in thousands)

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Underlying all potential applications of biotechnology to clean energy, mitigation of greenhouse gas effects on climate change, and environmental cleanup is the need for a solid understanding of the biochemistry and genetics of plants and microorganisms. We are only now beginning to appreciate the complexity of metabolic and regulatory signaling pathways in the simplest of bacteria that might be harnessed for clean energy and carbon management. Two simple examples: If, in the long-term, we are to enhance the productivity of forests, biomass crops and agricultural systems, it is imperative to understand why, for example, Rubisco--a mediator of photosynthesis and the single most abundant enzyme complex on Earth--is seemingly so energetically inefficient. This research program may show us that Rubisco can be engineered to carry out carbon fixation more efficiently, if its genetic regulatory circuits can be "rewired" or, perhaps, that there are more efficient forms of this enzyme still waiting to be discovered and used. Similarly, it may help to develop a more efficient hydrogen-based energy economy through an understanding of how oxygen poisons a key group of enzymes, hydrogenases, capable of producing hydrogen in the absence of air. This program will help us answer these types of questions.

The capture and sequestration of huge, gigaton volumes of carbon dioxide (CO<sub>2</sub>) on a global scale from power generation and heavy industry is central to the success of any future strategy to control atmospheric greenhouse gases. This research program contributes to this challenge through its systems approach to understand biological systems at both the molecular and environmental (microbial community) levels that can point to possible applications of this new knowledge. With an appropriate geologic energy source, subsurface microbial communities under thermodynamically favorable conditions might be manipulated to convert sequestered CO<sub>2</sub> into biomass, and ultimately extractable methane. This program will also seek to understand the need to understand microbiological and biogeochemical mechanisms important to long-term geologic storage and leakage of stored CO<sub>2</sub>.

Bioprocesses are often more energy efficient than current industrial processes. A key challenge, therefore, is to take advantage of and apply nature's efficiency to large-scale processing, a result that would help transform the energy economy. Bioconversion uses microorganisms such as bacteria and fungi or cell-free enzyme systems to capture energy or to transform organic or inorganic materials to useful products including fuel, food, fiber, and commodity and special chemicals. Heading the list of possibilities is the direct biological production of hydrogen and, perhaps in a simultaneous process, reducing the carbon density of coal, oil, and gas. Bioconversion also promises innovative approaches to clean energy and for mitigating greenhouse gas emissions by directly capturing emissions from industry and power generation. This program will provide the necessary knowledge base and the biotechnology tools to explore these possibilities.

Proteins rarely work alone. They assemble in larger multi-protein complexes often referred to as molecular machines. Understanding these molecular machines is a major goal of the research. Similarly, microbes of potential importance for DOE's energy and cleanup missions rarely work alone in nature. Microbes are often found as part of complex, and poorly understood consortia of many different types of microbes.



(dollars in thousands)

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The research will:

- Identify life's molecular machines, the multiprotein complexes that carry out the functions of living systems. Emphasis will focus on molecular machines from organisms of potential importance to DOE missions (e.g., energy production, environmental remediation, and carbon sequestration, and bioterror reduction).
- Characterize the gene regulatory networks and processes that control the molecular machines of interest.
- Characterize the functional repertoire of complex microbial communities in their natural environments and use the integrated genomics, biochemical, structural, and physiological information to address DOE missions in energy, waste cleanup, and bioterror reduction.
- Develop computational capabilities needed to model the complexity of biological systems.

The overriding goal of this long-term research program is to understand biology well enough to be able to predict the behavior and responses of biological systems – from cells to organisms so that they can best be used to address DOE mission needs in energy, the environment, and national security.

Computation and modeling of biological processes and systems is key to the success of this effort given the complexity of biological systems. Greatly improved computational strategies, tools and resources are needed and will be developed in partnership with the Advanced Scientific Computing Research program. One goal is to bring terascale computing into Genomes to Life as a model for all biologists.

The broad goals of this research are shared with other agencies, such as the National Institutes of Health and the National Science Foundation, and private sector companies and will require coordination exceeding that of the Human Genome Project. The program will focus on scientific challenges that can be uniquely addressed by DOE and its National Laboratories in partnership with scientists at universities and will focus on high throughput genomic-scale activities (e.g., DNA sequencing, complex computational analysis, and genomic protein-expression experimentation and analysis) that are out of reach of individual investigators or even small teams.

The increase in funding will accelerate development of the research infrastructure needed to conduct the complex, multidisciplinary research. Funds will be used to develop peer-reviewed, virtual, distributed research centers comprised of teams of National Laboratory, university, and private sector scientists who, together will develop, use, and distribute research resources for the program.

**Performance will be measured by:**

- The funding of new, large multidisciplinary research teams comprised of scientists from National Laboratories and universities and by the successful partnering with research programs in other federal agencies.
- In conjunction with ASCR, develop new computational tools for the analysis and simulation of biological processes.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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- For 3-5 of the over 70 microbial genomes sequenced by DOE, begin the difficult, comprehensive integration of genomic, biochemical, structural and physiological information on DOE relevant functionalities (e.g., bioremediation, carbon sequestration and/or biomass to fuel). Develop working conceptual and numerical models to describe these functionalities.
- Sequence one or more consortia of microorganisms that will provide information on how microbes function and interact in the environment, such as at DOE legacy waste sites.

■ **Human Frontiers Science** ..... **1,000**      **1,000**      **1,000**

BER will continue to fund the Human Frontiers Science program, an international program of collaborative research to understand brain function and biological function at the molecular level supported by the U.S. government through the DOE, the National Institutes of Health, the National Science Foundation, and the National Aeronautics and Space Administration. This program continues to get high marks from the international scientific community about the quality of the science it supports, the multidisciplinary and collaborative nature of the research and its productivity. In FY 2002, DOE expects to explore the possibility of other agencies with stronger interests in brain function continuing the program allowing DOE to refocus its efforts on more mission relevant science. FY 2003 funding will complete DOE activities.

■ **Low Dose Radiation Research** ..... **18,362**      **17,783**      **17,523**

The goal of the Low Dose Radiation Research program is to support research that will help determine health risks from exposures to low levels of ionizing radiation, information that is critical to adequately, and appropriately, protect people and to make the most effective use of our national resources.

In FY 2003, BER will continue to emphasize the use of new tools such as microbeam irradiators developed in the program in prior years, the characterization of individual susceptibility to radiation, and the forging of closer, more productive linkages between experimentalists and risk modelers, a relationship that lies at the critical interface between experimental science, risk analysis, and development of better risk management policies. In particular, research will focus on:

- *Bystander effect* – the response of cells that are not directly traversed by radiation but respond with gene induction and/or production of potential genetic and carcinogenic changes. It is important to know if bystander effects can be induced by exposure to low LET (linear energy transfer) radiation delivered at low total doses or dose-rates. This bystander effect potentially “amplifies” the biological effects (and the effective radiation dose) of a low dose exposure by effectively increasing the number of cells that experience adverse effects to a number greater than the number of cells directly exposed to radiation.
- *Genomic instability* – is the loss of genetic stability, a key event in the development of cancer, induced by radiation and expressed as genetic damage that occurs many cell divisions after the insult is administered. Current evidence suggests that DNA repair and processing of radiation damage can lead to instability in the progeny of irradiated cells and that susceptibility to

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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instability is under genetic control but there is virtually no information on the underlying mechanisms. Its role in radiation-induced cancer remains to be determined experimentally. It is also important to determine if genomic instability occurs at low total doses (<10 rads) or low dose rates.

- *Adaptive response* – is the ability of a low dose of radiation to induce cellular changes that reduce the level of subsequent radiation-induced or spontaneous damage. If low doses of radiation regularly and predictably induce a protective response in cells to subsequent low doses of radiation or to spontaneous damage, this could have a substantial impact on estimates of adverse health risk from low dose radiation. The generality and the extent of this apparent adaptive response needs to be quantified.
- *Endogenous versus low dose radiation induced damage* - A key element of the program will continue to investigate the similarities and differences between endogenous oxidative damage and damage induced by low levels of ionizing radiation as well as an understanding of the health risks from both. This information was not previously attainable because critical resources and technologies were not available. Today, technologies and resources such as those developed as part of the human genome program and at the National Laboratories have the potential to detect and characterize small differences in damage induced by normal oxidative processes and low doses of radiation.
- *Genetic factors that affect individual susceptibility to low dose radiation* – Research is also focused on determining whether genetic differences make some individuals more sensitive to radiation-induced damage since these differences could result in individuals or sub-populations that are at increased risk for radiation-induced cancer.
- *Mechanistic and risk models* – Novel research is supported that involves innovative collaborations between experimentalists and modelers to model the mechanisms of key radiation-induced biological responses and to describe or identify strategies for developing biologically-based risk models that incorporate information on mechanisms of radiation-induced biological responses.

Information developed in this program will provide a better scientific basis for making decisions with regard to remediating contaminated DOE sites and for determining acceptable levels of human health protection, both for cleanup workers and the public, in a more cost-effective manner. University scientists, competing for funds in response to requests for applications, conduct a substantial fraction of the research in this program.

**Performance will be measured:** By the end of FY 2003, results from the Low Dose Radiation Research program will be incorporated into the National Academy of Sciences Biological Effects of Ionizing Radiation (BEIR) VII report that will serve as a basis for future policy decisions on low dose radiation.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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■ <b>Congressional Direction</b> .....	<b>192</b>	<b>0</b>	<b>0</b>
Congressional direction in FY 2001 for a Study of Avian Populations at the Nevada Test Site.			
<b>Human Genome</b> .....	<b>85,491</b>	<b>87,858</b>	<b>90,185</b>
■ <b>Joint Genome Institute</b> .....	<b>61,822</b>	<b>57,200</b>	<b>57,200</b>

With the completion of the high quality DNA sequences of human chromosomes 16 and 19 in FY 2002 (DOE's share of the effort to sequence the human genome), the Joint Genome Institute (JGI) will continue to use its sequencing capacity to address the challenges of understanding the human genome, to address DOE mission needs and as a resource for our Nation's scientists. Past investments in DNA sequencing technology have continued to push costs down and throughput up making high-throughput DNA sequencing an even better scientific investment and a more effective research tool than ever for gene identification, finding gene regulatory elements, elucidating gene function, understanding evolutionary processes, developing the tools needed to predict cellular response to environmental stress, and performing the genetic manipulations needed to improve or alter gene function. In FY 2003 the JGI will focus on four main scientific areas:

- Microbial and Fungal Genomics
- Human Susceptibility
- Understanding the Regulatory Functions of DNA
- JGI as a National Resource

**MICROBIAL AND FUNGAL GENOMICS** – The JGI anticipates using 20% of its production DNA sequencing throughput on microbial and fungal genomics as well as a similar level of effort on functional genomics. The JGI will continue its efforts to understand the genomes and proteomes of microbial and fungal genomes important to DOE for:

- Carbon Sequestration - organisms that remove carbon from the environment
- Energy Sources - organisms that display novel photosynthetic or energy producing characteristics
- Bioremediation – organisms that act to clean up the environment
- Environmental Analysis - understanding how communities of microbes relevant to DOE missions interact to alter and detoxify their environment.
- Bioterrorism – organisms that could be used as or closely related to biothreat agents.

**HUMAN SUSCEPTIBILITY** - With the completion of the human DNA sequence we are now poised to understand how genes and the environment interact. This is especially important for understanding the role our genetic makeup plays in defining how we as individuals respond to

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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environmental stress in its many forms. This ties into many DOE programs, including the Low Dose Radiation Research program. The JGI will systematically analyze the human genome to first identify and then determine DNA sequence variation in the estimated ~5,000 human susceptibility genes. This will require an estimated 30% of the JGI production DNA sequencing capacity and the majority of its functional genomics resources. This information will be key to the Low Dose Radiation Research program with its complementary goal of understanding and characterizing genetic factors that contribute to individual sensitivity to energy-related insults.

**UNDERSTANDING THE REGULATORY FUNCTIONS OF DNA** - As a continuation of its responsibility to help understand the functioning of the human genome and as a key part of research on microbes for DOE energy and environmental needs, the JGI will focus on understanding the regulatory functions of DNA, such as gene regulation, characterization of DNA binding proteins and the full elucidation of gene promoters, enhancers and other regulatory mechanisms. Approximately 30% of the JGI's production DNA sequencing capacity will be required to meet this goal in addition to a proportion of its functional genomics resources. Model genomes currently under consideration for DNA sequencing and functional analysis to meet this goal include the *Ciona intestinalis*, chicken, and *Xenopus tropicalis*.

**JGI AS A NATIONAL RESOURCE** - A proportion, 20%, of the JGI's production DNA sequencing facility will be dedicated to the sequencing of a number of genomes or regions of interest as defined by the broader scientific community. This has proved to be a very productive and successful venture as demonstrated by previous "microbe months" in which large numbers of microbes were sequenced for JGI's scientific collaborators in a focused effort. The JGI will continue to seek guidance from its scientific advisors and to ensure that its efforts are of maximal benefit to DOE programs. Included in the JGI's DNA sequencing as a national resource is the completion of selected microbial and fungal genomes and a variety of projects in collaboration with and through grants from other agencies, such as the USDA.

**Performance will be measured by** (1) producing, with no increased funding, a total of approximately 8 billion base pairs of DNA sequence in FY 2003, a 100% increase in the number projected for FY 2001, and (2) establishing at least 30 diverse collaborations for high throughput DNA sequencing with scientists outside the JGI and with programs at other federal agencies.

- **Tools for DNA Sequencing and Sequence Analysis** ..... **21,242**    **28,179**    **30,280**

BER continues to develop the tools and resources needed by the scientific, medical, and private sector communities to fully exploit the information contained in the first complete human DNA sequence. Unimaginable amounts of DNA sequencing, at dramatically increased speed and reduced cost, will be required in the future for medical and commercial purposes and to understand the information in the DNA sequence that has already been determined. BER continues to support research to further improve the reagents used in DNA sequencing and analysis; to decrease the costs of sequencing; to increase the speed of DNA sequencing; and new computational tools for genome-wide data analysis. Novel sequencing strategies such as microchannel capillary electrophoresis offer great promise for the every day sequencing needs of the future.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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Use of sequence information to understand human biology and disease will also require new strategies and tools capable of high-throughput, genome-wide experimental and analytic approaches. In FY 2003, BER will continue to increase efforts to develop high-throughput approaches for analyzing gene regulation and function.

- Ethical, Legal, and Societal Issues (ELSI)** ..... **2,427**      **2,479**      **2,705**

The DOE and NIH human genome programs agreed at the outset to dedicate a fraction of their human genome program funding to understanding the ELSI issues associated with the genome program. DOE's ELSI research program represents 3 percent of the DOE human genome program. The DOE ELSI program supports research focused on issues of: (1) the use and collection of genetic information in the workplace especially as it relates to genetic privacy; (2) the storage of genetic information and tissue samples especially as it relates to privacy and intellectual property; (3) genetics and ELSI education; and (4) the ELSI implications of advances in the scientific understanding of complex or multi-genic characteristics and conditions.

A table follows displaying both DOE and NIH genome funding.

U.S. Human Genome Project Funding

(dollars in millions)

	Prior Years	FY 2001	FY 2002	FY 2003
DOE Total Funding (FY 87-00).....	779.0	85.5	87.9	90.2
NIH Funding (FY 88-00).....	1,859.2	382.4	426.7 <sup>a</sup>	TBD
Total U.S. Funding.....	2,638.2	467.9	514.6	TBD

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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**Health Effects**..... **17,616**      **13,640**      **14,251**

- Functional Genomics Research**..... **14,417**      **13,640**      **14,251**

*Scientific needs for functional genomics research* - Functional genomics research capitalizes on our understanding and the manipulability of the genomes of model organisms, including Fugu (puffer fish), Ciona (sea squirt), and mouse, to speed understanding of human genome organization, regulation, and function. This research is a key link between human genomic sequencing, which provides a complete parts list for the human genome, and the development of information (a high-

<sup>a</sup> Estimate from NIH.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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tech owner’s manual) that is useful in understanding normal human development and disease processes. The mouse continues to be a major focus of our efforts. It is an integral part of our functional genomics research effort. BER creates and genetically characterizes new mutant strains of mice that serve as important models of human genetic diseases and for understanding gene function. It also develops high-throughput tools and strategies to characterize these mutant strains of mice. This mouse genetics research provides tools useful to the entire scientific community for decoding the functionality of the human genome as human DNA sequence becomes available. Research to develop new strategies for using model organisms such as the mouse, Fugu, and *Ciona* to understand the function of human genes continues in FY 2003.

<ul style="list-style-type: none"> <li> <b>Technology Development Research</b> .....           <span style="float: right;">3,199</span> <span style="float: right;">0</span> <span style="float: right;">0</span> </li> </ul>			
Technology development research is absorbed within the individual Life Sciences subprogram elements .....			
<b>SBIR/STTR</b> increased with Life Sciences program increase .....	<b>0</b>	<b>4,876</b>	<b>5,331</b>
<b>Total, Life Sciences</b> .....	<b>188,469</b>	<b>192,573</b>	<b>210,878</b>

In FY 2001 \$4,329,000 and \$260,000 were transferred to the SBIR and STTR programs, respectively. FY 2002 and FY 2003 amounts are estimated requirements for the continuation of these programs.

### Explanation of Funding Changes from FY 2002 to FY 2003

FY 2003 vs. FY 2002 (\$000)
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#### Structural Biology

- Maintain structural biology research at near FY 2002 levels..... -80

#### Molecular and Cellular Biology

- Increase for Genomes to Life research on microbes that work to address DOE needs focused on understanding cellular processes and multicellular systems to a level where predictive simulation models can be developed to guide the use or development of microbial systems to solve DOE mission needs for energy use and production, waste cleanup, carbon sequestration, and biothreat reduction; and maintain microbial genomics and carbon sequestration research at near FY 2002 levels..... +15,252
  - Maintains Low Dose Radiation Research at near FY 2002 levels..... -260
- Total, Molecular and Cellular Biology..... +14,992

FY 2003 vs. FY 2002 (\$000)
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**Human Genome**

<ul style="list-style-type: none"> <li>■ High throughput sequencing to characterize the function and regulation of genes on human chromosomes 5, 16, 19 (the chromosomes worked on by DOE) and to use high throughput sequencing as a basic research tool in biology.....</li> </ul>	+2,101
<ul style="list-style-type: none"> <li>■ Ethical, Legal, and Societal Issues program maintains funding at approximately 3% of total human genome funding .....</li> </ul>	+226
<hr/>	
Total, Human Genome .....	+2,327

**Health Effects**

<ul style="list-style-type: none"> <li>■ Increase for research that develops strategies and tools to understand human gene function using model organisms. ....</li> </ul>	+611
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**SBIR/STTR**

Increase in SBIR/STTR due to increase in research funding for the Life Sciences program. ....	+455
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Total Funding Change, Life Sciences .....	+18,305



# Climate Change Research

## Mission Supporting Goals and Objectives

The goal of the Climate Change Research subprogram (previously the Environmental Processes subprogram) is to deliver relevant scientific knowledge that will enable scientifically-based predictions and assessments of the potential effects of greenhouse gas and aerosols emissions on climate and the environment. Research will reduce and resolve key uncertainties and provide the scientific foundation needed to predict, assess, and mitigate adverse effects of energy production and use on the environment through research in climate modeling and simulation, climate processes, carbon cycle and carbon sequestration, atmospheric chemistry, and ecological science.

The Climate Change Research subprogram supports four contributing areas of research: Climate and Hydrology; Atmospheric Chemistry and Carbon Cycle; Ecological Processes; and Human Interactions. The research is focused on understanding the physical, chemical, and biological processes affecting the Earth's atmosphere, land, and oceans and how these processes may be affected, either directly or indirectly, by energy production and use, primarily the emission of carbon dioxide from fossil fuel combustion. BER has designed and planned the research program to provide the data that will enable objective assessments of the potential for, and consequences of, global warming. The BER Climate Change Research subprogram (excluding the carbon sequestration element) represents DOE's contribution to the interagency U.S. Global Change Research Program proposed by President Bush in 1989 and codified by Congress in the Global Change Research Act of 1990 (P.L. 101-606). The National Institute for Global Environmental Change (NIGEC) is integrated throughout the subprogram (FY 2003 Request is \$8,763,000).

A major emphasis of the Climate Change Research subprogram is on understanding the radiation balance from the surface of the Earth to the top of the atmosphere and how changes in this balance due to increases in the concentration of greenhouse gases in the atmosphere may alter the climate. Much of the research is focused on improving the quantitative models necessary to predict possible climate change at global and regional scales. Research in the Atmospheric Radiation Measurement (ARM) program will continue to focus on resolving the greatest scientific uncertainty in climate change prediction – the role of clouds and solar radiation. ARM seeks to develop a better quantitative understanding of how atmospheric properties, including the extent and type of cloud cover and changes in aerosols and greenhouse gas concentrations affect the solar and infrared radiation balance that drives the climate system. BER's Climate Modeling program develops advanced, fully coupled climate models and uses massively parallel supercomputers to simulate and predict climate and climate change, including evaluating uncertainties in climate models due to changes in atmospheric levels of greenhouse gases on decade-to-century time scales.

The Atmospheric Science program is focused on acquiring the data to understand the atmospheric processes that control the transport, transformation, and fate of energy-related chemicals and particulate matter emitted to the atmosphere. BER is emphasizing research on processes relating to new air quality standards for tropospheric ozone and particulate matter and relationships between air quality and climate change.

Research on the carbon cycle explores the movement of carbon on a global scale starting from natural and anthropogenic emissions to ultimate sinks in the terrestrial biosphere and the oceans. Experimental and modeling efforts primarily address the net exchange of carbon between major types of terrestrial ecosystems and the atmosphere. This research includes DOE's contribution to the Climate Change Research Initiative, an interagency effort on specific areas of climate change research in which substantial progress in understanding and modeling is expected over the next five years.

The BER carbon sequestration research funds basic research that seeks to exploit the biosphere's natural processes to enhance the sequestration of atmospheric carbon dioxide in terrestrial and marine ecosystems. It also seeks the understanding needed to assess the potential environmental implications of purposeful enhancement and/or disposal of carbon in the terrestrial biosphere and at the surface or deep ocean. The carbon sequestration activities include research to identify and understand the environmental and biological factors or processes that limit carbon sequestration in these systems and to develop approaches for overcoming such limitations to enhance sequestration. The research includes studies on the role of ocean and terrestrial microorganisms in carbon sequestration.

The Ecological Processes research is focused on experimental and modeling studies to understand and simulate the effects of climate and atmospheric changes on the biological structure and functioning of terrestrial ecosystems. The research also seeks to identify the potential feedback effect of ecosystem responses on climate and atmospheric composition. The research emphasizes major field studies of intact ecosystems using experimental manipulations of, for example, carbon dioxide and ozone concentrations and precipitation, and using data from these experiments to develop, test, and improve models for simulating and predicting ecosystem responses.

The Human Interactions research is focused on improving methods and models that can be used to assess the economic and societal costs and benefits of both human-induced climate change and possible response options or strategies for mitigating or adapting to climate change. It also includes support to archive and analyze global change data and make it available for use by the broader global change research community.

### Funding Schedule

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
Climate and Hydrology.....	71,205	70,490	74,669	+4,179	+5.9%
Atmospheric Chemistry and Carbon Cycle .....	35,193	34,666	37,764	+3,098	+8.9%
Ecological Processes.....	11,352	12,383	13,888	+1,505	+12.2%
Human Interaction.....	7,928	8,054	8,084	+30	+0.4%
SBIR/STTR .....	0	3,329	3,554	+225	+6.8%
<b>Total, Climate Change Research .....</b>	<b>125,678</b>	<b>128,922</b>	<b>137,959</b>	<b>+9,037</b>	<b>+7.0%</b>

## Detailed Program Justification

(dollars in thousands)

	FY 2001	FY 2002	FY 2003
<b>Climate and Hydrology</b> .....	<b>71,205</b>	<b>70,490</b>	<b>74,669</b>
<ul style="list-style-type: none"> <li> <span style="display: inline-block; width: 1em; height: 1em; background-color: black; margin-right: 0.5em;"></span> <b>Climate Modeling</b>.....           <span style="float: right; text-align: right;"> <b>27,301</b>    <b>27,064</b>    <b>27,181</b> </span> </li> </ul>			

Model based climate prediction provides the most scientifically valid way of predicting the impact of human activities on climate for decades to centuries in the future. BER will continue to develop, improve, evaluate, and apply the best coupled atmosphere-ocean general circulation models (GCMs) that simulate climate variability and climate change over these time scales. The goal is to achieve statistically accurate forecasts of future climate over regions as small as river basins using ensembles of model simulations. The ensembles will accurately incorporate the dynamic and thermodynamic feedback processes that influence climate, including clouds, aerosols, and greenhouse gas forcing. Current predictions are limited by the inadequacy of computational resources and uncertainties in the model representations of key small-scale physical processes, especially those involving clouds, evaporation, precipitation, and surface energy exchange. BER will address both the computational and scientific shortcomings through an integrated effort. Support will continue to be provided to acquire the high-end computational resources needed to complete ensembles of climate simulations using present and future models. BER will emphasize research to develop and employ information technologies that can quickly and efficiently work with large and distributed data sets of both observations and model predictions to produce quantitative information suitable for the study of regional climate changes. BER will continue to fund the multi-institutional research consortia established in FY 2001 to further the development of comprehensive coupled GCMs for climate prediction that are of higher resolution and contain accurate and verified representations of clouds and other important processes.

**Performance will be measured:** By the end of FY 2003, the program will increase the realism of the parallel coupled climate model by increasing the spatial resolution of the atmospheric model to 1.4 degrees and the ocean and sea ice model to approximately 0.7 degrees, which will be a higher resolution than any fully coupled climate model currently available to assess climate change. The capacity to produce multiple, long-term climate change scenarios for climate change research and assessment purposes will be enhanced by improvements in computing software and the development of improved algorithms needed to effectively exploit the new computing technology.

In FY 2003, BER will continue the partnership with the Advanced Scientific Computing Research program. This includes applying the computing resources for climate simulation and continuing climate model development and application through the use of collaborative technologies. Additionally, BER will increase the emphasis on data assimilation methods so as to quickly make use of the high quality observational data streams provided by ARM, satellite and other USGCRP climate data programs to evaluate model performance.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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NIGEC will continue the support of research to evaluate the reliability of using isotopic signatures of trace gases in ice cores for interpreting climate variation and change in the past and the relationship between greenhouse gas concentrations and climate change (FY 2003 Request is \$2,191,000).

■ **Atmospheric Radiation Measurement (ARM) Research .....**      **13,812    13,310    13,310**

The principal goal of the ARM scientific enterprise is to develop an improved understanding of the radiative transfer processes in the atmosphere and to formulate better parameterizations of these processes in climate prediction models, referred to as General Circulation Models (GCMs). ARM research supports about 50 principal investigators involved in studies of cloud physics and the interactions of solar and infrared radiation with water vapor and aerosols (including black soot). University scientists form the core of the ARM science team that networks with the broader academic community as well as with the scientists at the DOE National Laboratories and with federal scientists at NASA, NOAA, and DOD. ARM scientists pursue research as individuals and as members of teams and contribute both to the production of ARM data, e.g., as designers of cutting-edge remote sensing instrumentation, as well as consumers of the data produced at the three ARM sites. To facilitate the knowledge transfer from the ARM program to the premier modeling centers, the ARM program supports scientific "Fellows" at the NSF's National Center for Atmospheric Research, the NOAA's National Center for Environmental Prediction, and the European Center for Medium-Range Weather Forecasting in the U.K.

**Performance will be measured:** By the end of FY 2003, the program will deliver a more realistic representation of clouds for incorporation in atmospheric general circulation models. The improved representation of clouds will result in a 10% reduction in the uncertainty in calculations of the atmospheric energy budget and improve the accuracy and precision of climate models used to simulate and predict the effects on climate of atmospheric increases in energy-related greenhouse gases and aerosols.

■ **Atmospheric Radiation Measurement (ARM) Infrastructure..**      **27,371    27,371    31,441**

The Atmospheric Radiation Measurement (ARM) infrastructure program develops, supports, and maintains the three ARM sites and associated instrumentation. BER will continue to operate over two hundred instruments (e.g., multifilter shadowband radiometers for aerosol measurements, Raman Lidar for aerosol and cloud measurements, radar wind profiler systems, radar cloud measurement systems, sky imaging systems, arrays of pyranometers, pygeometers, and pyrhemometers for atmospheric and solar radiation measurements, and standard meteorological measurement systems for characterization of the atmosphere) at the Southern Great Plains site and will continue operations at the Tropical Western Pacific station and at the North Slope site in Alaska. The ARM program will continue to provide data to the scientific community through the ARM Archive.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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The ARM data streams will continue to be enhanced periodically by additional measurements at the ARM sites during intensive field campaigns referred to as Intensive Operation Periods (IOP). Ranging from two weeks to two months, the campaigns bring together teams of scientists testing cutting edge remote sensing instruments and coordinate measurements with airborne and satellite observations. The ARM sites have become major testbeds of research in atmospheric processes serving as scientific user facilities for hundreds of scientists from universities and government laboratories. For example, both DOD and NASA have used the ARM sites to "ground truth" their satellite instruments.

The increased funding will provide new instrumentation at the three ARM sites to measure the major components of the water cycle (including atmospheric water vapor, precipitation, evaporation, transpiration, soil water, and water runoff from land surfaces) and to measure energy-related aerosols and their radiative properties. The water cycle measurements will improve the climate models' parameterization of the coupling of radiation, cloud processes, and the land surface processes to reduce the current high uncertainty in predictions of precipitation patterns. The new knowledge gained from the water cycle study and aerosol measurements is important for climate studies. Additional staff and equipment will be provided to the ORNL ARM Data Archive to quality assure and distribute the data. The investment will increase the ARM users from about 680 to 800.

**Performance will be measured** by achieving a downtime of less than five percent for the principal ARM instruments and by the successful conduct of five IOPs across the three ARM sites.

- **Atmospheric Radiation Measurement (ARM)/Unmanned Aerial Vehicles (UAV)**..... **2,721**      **2,745**      **2,737**

The UAV program will conduct one major field campaign in conjunction with the ARM program to provide high altitude measurements of cloud properties and radiation budget.

- Atmospheric Chemistry and Carbon Cycle**..... **35,193**      **34,666**      **37,764**

- **Atmospheric Science** ..... **14,582**      **12,510**      **12,571**

The Atmospheric Science projects acquire data to understand the atmospheric processes that control the transport, transformation, and fate of energy-related chemicals and particulate matter. Emphasis is placed on processes relating to new air quality standards for tropospheric ozone and particulate matter and relationships between air quality and climate change. Field and laboratory studies will continue to be conducted in both atmospheric chemistry and environmental meteorology and acquired data will be used to develop and validate predictive models of atmospheric processes. The research will include studies of chemical and physical processes affecting air pollutants such as sulfur and nitrogen oxides, tropospheric ozone, gas-to-particle conversion processes, and the deposition and resuspension of associated aerosols. It also includes studies to improve understanding of the meteorological processes that control the dispersion of energy-related chemicals and particulates in the atmosphere. Much of this effort involves multi-agency collaboration, and university scientists play key roles. New information will document both the contribution of energy production to regional haze in the U.S. and the relationship between urban and regional air pollution

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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processes and continental, intercontinental, and global scale phenomena. The information is essential for assessing the effects of energy production on air quality and will contribute to the evaluation of science-based options for minimizing the impact of energy production on visibility.

In FY 2003 BER will continue the Tropospheric Aerosol Program (TAP) to quantify the impacts of energy-related aerosols on climate, air quality, and human health. TAP will be closely coupled with other components of DOE’s global change research, especially the Atmospheric Radiation Measurement (ARM) program. TAP will also be broadly coordinated with the air quality and global change research communities, including collaborations with the EPA, NASA, and NOAA and with the DOE Office of Fossil Energy’s Airborne Fine Particulate Matter (PM) Research program. Regional patterns of aerosol distribution will be related to sources and sinks and the information will feed the models that simulate the impacts of aerosols on air quality and climate.

In FY 2003 the Atmospheric Sciences subprogram will, in general, focus on the evaluation of preliminary findings from field measurement campaigns in both atmospheric chemistry and environmental meteorology.

**Performance will be measured** by the extent, over five years, to which scientific results are incorporated into models to predict and assess air quality and radiative forcing of other energy-related greenhouse gases (such as ozone) and aerosols.

NIGEC will support research to quantify the effects of natural processes on atmospheric composition, including the exchange of energy-related trace gases between the atmosphere and the terrestrial biosphere (FY 2003 Request is \$2,191,000).

■ **Terrestrial Carbon Processes and Ocean Sciences..... 10,557 13,635 13,716**

BER will continue supporting the AmeriFlux program, which is a network of approximately 25 research sites where the net exchange of CO<sub>2</sub>, energy, and water between the atmosphere and major terrestrial ecosystems in North America. These measurements are linked to field measurement campaigns across North America that will test how well point measurements represent larger areas and allow the estimation of carbon sources and sinks on a regional basis. This research supports the interagency Carbon Cycle Science Plan. The fluxes of other greenhouse gases, e.g., methane and nitrous oxide, will also be measured at several AmeriFlux sites.

BER will also continue research to refine and test carbon cycle models (based on mechanistic representations and simple carbon accounting). The models will be used to estimate potential carbon sequestration in response to changes in environmental factors, including climate.

**Performance will be measured:** By the end of FY 2003, the program will deliver quantitative estimates of net annual carbon sequestration in terrestrial ecosystems at five of the AmeriFlux network sites. The program will also deliver regional-scale estimates of the terrestrial carbon budget for three regions in North America such as the deciduous forest region of the eastern U.S.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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The focus of the ocean science element is on using microbiology tools to determine the linkages between the carbon and nitrogen cycles involving marine microbes. This research is conducted through partnerships between institutions with a tradition of research in oceanography (such as Skidaway Institute of Oceanography, U. of Washington, U. of Delaware, Rutgers University, U. of South Florida, Princeton University), and institutions traditionally serving minority students (such as Lincoln U., Howard U., Savannah State U., U. of Puerto Rico, and San Francisco State).

■ **Climate Change Research Initiative** ..... **0**      **0**      **2,920**

In FY 2003, the Administration will institute a new Climate Change Research Initiative (CCRI). The set of cross agency programs with a strong focus on outcomes and deliverables. The CCRI will focus on specific areas of research, including climate variation and change, carbon cycle, water cycle, atmospheric composition, and regional impacts. DOE, in conjunction with other USGCRP agencies, e.g., NASA, NOAA, NSF, etc., will contribute to one specific research area. The deliverables will be targeted at information useful to policy-makers, such as more reliable predictions of what the future climate would be under different greenhouse forcing scenarios and how much climate and land use changes will affect natural sources and sinks of carbon. DOE will participate in one of the specific research areas: understanding the North American Carbon Cycle (with NOAA, NSF, and USDA), which is identified as a priority need in the interagency Carbon Cycle Science Plan.

BER activities on the carbon cycle explore the movement of carbon on a global scale starting from natural and anthropogenic emissions to ultimate sinks in the terrestrial biosphere and the oceans. The AmeriFlux sites are essential to quantifying the net exchange of carbon between the atmosphere and major terrestrial ecosystems in North America and hence are essential to documenting the magnitude and variation in the North American carbon sink and how it is affected by interannual changes in climate. Experimental and modeling efforts primarily address the net exchange of carbon between major types of terrestrial ecosystems and the atmosphere.

BER will expand the facilities in the successful AmeriFlux program by including intensive measurements of additional parameters (e.g., above and belowground carbon stocks in roots, soil organic matter, aboveground tree trunks, stems leaves, litter, etc., and mortality of vegetation) and processes (e.g., photosynthesis, plant and microbial respiration rates, decomposition rate, carbonic acid weathering rate (which consumes CO<sub>2</sub>), and vegetation growth rate) at the existing 25 AmeriFlux sites across North America and extensive measurements that transcend larger areas surrounding these sites, thereby allowing the estimation of carbon sources and sinks at landscape and regional scales. This information will provide a sound scientific basis for extrapolating carbon flux measurements at AmeriFlux sites to regional and continental scales and hence, improve estimates of both the magnitude of the North American carbon sink and the major terrestrial ecosystems that account for the sink. Fluxes of other greenhouse gases, including methane, nitrous oxide, and water vapor will also be measured at several AmeriFlux sites. The investment will increase the number of users from about 125 to 200.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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- **Congressional Direction** ..... 1,725            0            0
- **Carbon Sequestration Research** ..... 8,329            8,521            8,557

BER will continue support for one carbon sequestration research consortium, led by ORNL, PNNL, and ANL, and involving six collaborative universities, that focuses on terrestrial sequestration (\$3,000,000). The consortium develops the information to enhance the natural sequestration of carbon in terrestrial soils and vegetation. BER will also continue the support of research at universities and DOE laboratories on ocean carbon sequestration (\$2,000,000). The focus of the research on terrestrial and ocean sequestration will continue to be on cellular and biogeochemical processes that control the rate and magnitude of carbon sequestration in terrestrial and oceanic systems, including the identification of pathways and processes that could be modified to enhance the net flow of carbon from the atmosphere to terrestrial plants and soils, and to the ocean surface and, ultimately, to the deep ocean. Also, BER will support the research needed to assess the environmental implications of enhancing carbon sequestration and storage in the ocean and in terrestrial systems. BER research on carbon sequestration in terrestrial ecosystems will improve the scientific understanding of mechanisms of sequestration and how to alter them to enhance sequestration. The Carbon Sequestration in Terrestrial Ecosystems (CSiTE) activity will conduct research that specifically examines those plant and soil processes that capture and retain carbon in chemical and physical forms that are resistant to decay. The data will inform new models for estimating carbon sequestration in terrestrial ecosystems. New technologies will be successfully developed by the BER-supported ocean carbon sequestration research to facilitate the export of carbon to the deep ocean and for re-mineralization of organic carbon at depth. Such technologies are vital to assessing accurately the potential of enhancing ocean carbon sequestration. Initial *in situ* experiments will be designed to determine the feasibility and potential environmental impacts of deep ocean injection of carbon dioxide (CO<sub>2</sub>). Associated research will include determination of chemical reactions at depth, stability of products, and effects of those products on marine organisms.

**Performance will be measured** by applying an ecosystem framework to estimate annual rates of actual carbon gain by vegetation and soil, and enhanced sequestration will be estimated relative to baseline carbon quantities established for the range of ecosystems investigated by the CSiTE.

In FY 2003 university scientists will continue research on the effects of iron fertilization on plankton communities in the ocean and begin field experiments. The ocean surrounding Antarctica is the largest high-nutrient, low-chlorophyll region in the world. The joint DOE-NSF Southern Ocean Iron Enrichment Experiment (SoFEX) will help scientists understand the potential to enhance ocean carbon sequestration through iron enrichment.



(dollars in thousands)

FY 2001	FY 2002	FY 2003
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**Performance will be measured by** the analysis and publication of results from the Southern Ocean Iron Fertilization Experiment (SOFeX) which will study the export of particulate organic carbon below the mixed layer in high and low silicate waters following the experimental addition of iron to a large area of the surface ocean, delivering data necessary to understand and assess the efficacy of using iron fertilization to enhance carbon sequestration in the ocean.

**Ecological Processes** ..... **11,352**      **12,383**      **13,888**

BER will continue the six Free-Air Carbon Dioxide Enrichment (FACE) experiments at Maricopa, Arizona; Cedar Creek Natural History Area, Minnesota; Duke University, Durham, North Carolina; Rhinelander, Wisconsin; Mercury, Nevada; and Oak Ridge, Tennessee (ORNL) to improve understanding of the direct effects of elevated carbon dioxide and other atmospheric changes on the structure and functioning of various types of terrestrial ecosystems, including coniferous and deciduous forests, grasslands, and desert. Increasing emphasis will be on evidence of differential responses of plant species that may impact plant competition, succession, and productivity in terrestrial ecosystems. Research will explore changes, over time, in the elevated productivity of terrestrial plants exposed to elevated atmospheric carbon dioxide (CO<sub>2</sub>) concentrations.

The long-term experimental investigation at the Walker Branch Watershed in Tennessee will continue to improve the understanding of the direct and indirect effects of alterations in the annual average precipitation on the functioning and structure of a southeastern deciduous forest ecosystem.

Both the FACE network and the Walker Branch Watershed represent scientific user facilities that have attracted scientists from both the academic community and government laboratories who use the facilities to develop new instrument methodologies and test scientific hypotheses related to ecosystem responses, including carbon sequestration, to climate and atmospheric changes.

Currently, the number of users conducting research at FACE facilities is affected by increased operational costs (e.g., cost of gases, electricity, security, and maintenance, replacement, and upgrade of instruments and other infrastructure at these facilities). The FY 2003 investment will provide the operational resources needed to effectively and efficiently maintain planned operation of the FACE facilities, thereby ensuring the facilities are maintained and operated in a way that benefits and attracts users and supports their needs. This investment in FACE facility operations will allow an increase in the number of users from about 200 in FY 2002 to 300 in FY 2003.

**Performance will be measured by** completion of a synthesis of data collected during 8-9 years of a unique experimental manipulation of precipitation received by a large-statured forest on the Oak Ridge reservation in a published book. This will include using the data collected in the experiment to evaluate (test) up to 15 ecosystem models for use in assessing forest responses to alterations in precipitation resulting from climate change.

NIGEC will support experimental studies to document how climate warming and increasing CO<sub>2</sub> levels in the atmosphere affect biophysical processes in terrestrial ecosystems (FY 2003 Request is \$2,629,000).

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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<b>Human Interactions</b> .....	<b>7,928</b>	<b>8,054</b>	<b>8,084</b>
■ <b>Human Interactions</b> .....	<b>7,928</b>	<b>8,054</b>	<b>8,084</b>

The Integrated Assessment program, with a strong academic involvement, will continue to support research that will lead to better estimates of the costs and benefits of possible actions to mitigate global climate change. The new emphasis will be to improve the integrated assessment models to include other greenhouse gases as well as carbon dioxide, carbon sequestration, and international trading of emission permits. The models will better represent the efficiency gains and losses of alternate emission reduction plans, including market adjustments to inter-regional differences among relative energy prices, regulations, and production possibilities in the international arena. Integrated assessment models will be modified to include carbon sequestration as an alternative mitigation option. This representation will include both options to enhance natural carbon storage in the terrestrial biosphere, as well as engineering options, such as the capture of carbon dioxide and storage in geologic formations.

The research will include integrating a new land and ocean carbon sub-model in a large integrated assessment model. The submodel includes a detailed representation of direct human influence (mainly agriculture and forestry) on the terrestrial biosphere. In addition to providing a more accurate representation of the global carbon cycle, the change will ensure consistent accounting of carbon-sink projects and the carbon uptake that occurs as a result of other land-use change and the effects of climate change and carbon fertilization. A second integrated assessment model will be used to simulate the effect of 1) climate on crop yields and 2) the amount of crop and pasture land necessary to provide a) a sufficient diet in developing countries under climate change and b) the likely increase in dietary requirements as developing countries become richer.

NIGEC will support research to develop and test new methods involving the use of large regional databases and coupled climate-impact-economic models to conduct integrated assessments of the effects of climate change on regionally important resources in the U.S. (FY 2003 Request is \$1,752,000).

The Information and Integration element stores, evaluates, and quality-assures a broad range of global environmental change data, and disseminates these to the broad research community. BER will continue the Quality Systems Science Center for the tri-lateral (Mexico, United States, and Canada) NARSTO (formally known as the North American Strategy for Tropospheric Ozone), a public partnership for atmospheric research in support of air quality management. The Center serves a diverse set of users, including academic and laboratory scientists and policy makers across North America.

The Global Change Education program supports DOE-related research in global environmental change for both undergraduate and graduate students, through the DOE Summer Undergraduate Research Experience (SURE), the DOE Graduate Research Environmental Fellowships (GREF), and collaboration with the NSF Significant Opportunities in Atmospheric Research and Science (SOARS) program.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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**Performance will be measured** by sustaining the number, quality, and diversity of students enrolled in the program and by end-of-summer evaluations by students and their mentors.

<b>SBIR/STTR</b> .....	<b>0</b>	<b>3,329</b>	<b>3,554</b>
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In FY 2001 \$3,160,000 and \$188,000 were transferred to the SBIR and STTR programs, respectively. FY 2002 and FY 2003 amounts are estimated requirements for the continuation of these programs.

<b>Total, Climate Change Research</b> .....	<b>125,678</b>	<b>128,922</b>	<b>137,959</b>
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### Explanation of Funding Changes from FY 2002 to FY 2003

FY 2003 vs. FY 2002 (\$000)
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#### Climate and Hydrology

- Climate modeling continued at near FY 2002 level..... +117
  - The ARM increase in funding will support new instrumentation and ARM site staff for additional user support at the ARM sites and ARM data archive to allow the replacement and maintenance of ARM instruments and needed user support for scientists who use the ARM data or the ARM sites for field research. .... +4,070
  - Unmanned Aerial Vehicle (UAV) continued at near FY 2002 level. .... -8
- |                                   |        |
|-----------------------------------|--------|
| Total, Climate and Hydrology..... | +4,179 |
|-----------------------------------|--------|

#### Atmospheric Chemistry and Hydrology

- Atmospheric science continued at near FY 2002 level..... +61
  - Terrestrial Carbon Process and Ocean Sciences continued at near FY 2002 levels. .... +81
  - BER will participate in the Climate Change Research Initiative research area to understand the North American carbon cycle by expanding the AmeriFlux network of research sites to allow regional extrapolation of net carbon exchange measurements..... +2,920
  - Carbon Sequestration Research Consortia continued at near FY 2002 level..... +36
- |  |        |
|--|--------|
| Total, Atmospheric Chemistry and Hydrology ..... | +3,098 |
|--|--------|

FY 2003 vs. FY 2002 (\$000)
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**Ecological Processes**

- The increase will support core operational costs at FACE sites to allow additional users at the sites by enabling the sites to be operated and maintained so as to attract a broader community of scientific users. .... +1,505

**Human Interactions**

- Human Interactions research is continued at near FY 2002 levels. .... +30

**SBIR/STTR**

Increase in SBIR/STTR due to increased research funding for Climate Change Research. .... +225

Total Funding Change, Climate Change Research..... +9,037

# **Environmental Remediation**

## **Mission Supporting Goals and Objectives**

The goal of the Environmental Remediation subprogram is to deliver relevant scientific knowledge that advances novel biotechnology solutions for environmental cleanup operations. Research on modified microbial processes that can stabilize radioactive waste and other toxic pollution in place, will contribute to remediation and restoration of contaminated environments at DOE sites and may also improve processes for recovery of valuable metals and production of fuel stocks.

BER's research in environmental remediation is focused on gaining improved understanding of the fundamental biological, chemical, geological, and physical processes that must be marshaled for the development and advancement of new, effective, and efficient processes for the remediation and restoration of the Nation's nuclear weapons production sites. Research priorities are on bioremediation and on operation of the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL).

Bioremediation activities are centered on the Natural and Accelerated Bioremediation Research (NABIR) program, a basic research program focused on determining how and where bioremediation may be applicable as a reliable, efficient, and cost-effective technique for cleaning up or containing metals and radionuclides in contaminated subsurface environments. In this subprogram, BER also includes basic research in support of pollution prevention, sustainable technology development and other fundamental research to address problems of environmental contamination.

In the NABIR program, research advances will continue to be made from molecular to field scales in the Biogeochemical Dynamics element; on genes and proteins used in bioremediation through the Biomolecular Science and Engineering element; in non-destructive, real-time measurement techniques in the Assessment element; in overcoming physico-chemical impediments to bacterial activity in the Acceleration element; on species interaction and response of microbial ecology to contamination in the Community Dynamics and Microbial Ecology element; and in understanding microbial processes for altering the chemical state of metallic and radionuclide contaminants through the Biotransformation element. In analogy with the Ethical, Legal, and Social Implications component of the Human Genome program, the Bioremediation and its Societal Implications and Concerns component of NABIR is exploring societal issues surrounding bioremediation research and promoting open and interactive communication with affected stakeholders to help ensure understanding and acceptance of bioremediation as a potential solution to remediating contaminants. All NABIR elements and EMSL activities have a substantial involvement of academic scientists.

Clean up research activities include a modest program in clean up research that will characterize the geologic, chemical, and physical properties that affect the rate and effectiveness of a variety of environmental remediation and waste-stream cleanup methods, including bioremediation; the Environmental Management Science Program, a cooperative program with the Office of Environmental Management to provide the science to solve the cleanup problems of the Nation's nuclear weapons complex; and ecological research conducted at the Savannah River Ecology Laboratory. The latter two activities are transferred in FY 2003 from Environmental Management to the Biological and Environmental Research program.

Within Facility Operations, support of the operation of the EMSL national user facility is provided for basic research that will underpin safe and cost-effective environmental remediation methods and technologies, other environmental science endeavors, and national security. Unique EMSL facilities, such as the Molecular Science Computing Facility, the High-Field Mass Spectrometry Facility, and the High-Field Magnetic Resonance Facility, are used by the external scientific community and EMSL scientists to conduct a wide variety of molecular-level environmental science research, including improved understanding of chemical reactions in DOE's underground storage tanks, transport of contaminants in subsurface groundwater and vadose zone sediments, and atmospheric chemical reactions that contribute to changes in the atmospheric radiative balance.

BER's William R. Wiley Environmental Molecular Sciences Laboratory will use its capabilities to expand its collaborations in the areas of structural biology and functional genomics. The number of users undertaking structural biology research will also increase.

### Funding Schedule

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
Bioremediation Research.....	27,538	27,997	30,700	+2,703	+9.7%
Clean Up Research.....	45,449	47,502	38,190	-9,312	-19.6%
Facility Operations .....	31,248	37,333	37,948	+615	+1.6%
SBIR/STTR .....	0	1,569	2,692	+1,123	+71.6%
<b>Total, Environmental Remediation .....</b>	<b>104,235</b>	<b>114,401</b>	<b>109,530</b>	<b>-4,871</b>	<b>-4.3%</b>

### Detailed Program Justification

(dollars in thousands)

	FY 2001	FY 2002	FY 2003
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**Bioremediation Research..... 27,538 27,997 30,700**

■ **NABIR and Bioremediation Research ..... 21,571 22,042 24,720**

NABIR will increase the understanding of the intrinsic bioremediation (natural attenuation) of DOE relevant metal and radionuclide contaminants, as well as of manipulated, accelerated bioremediation using chemical amendments. Laboratory and field experiments will be conducted to explore the fundamental mechanisms underlying chemical processes and complexation/transformation of contaminants. The NABIR Field Research Center is in operation at the Oak Ridge National Laboratory. Field site characterization of this Field Research Center and distribution of research samples to investigators will continue. In FY 2003, science elements in the NABIR program include fundamental research in the following subjects: (1) Biotransformation (microbiology to elucidate the mechanisms of biotransformation of metals and radionuclides); (2) Community Dynamics and Microbial Ecology (structure and activity of subsurface microbial communities); (3) Biomolecular Science and Engineering (molecular and structural biology to enhance the understanding of

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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bioremediation and identify novel remedial genes); (4) Biogeochemical Dynamics (dynamic relationships among *in situ* geochemical, geological, hydrological, and microbial processes); (5) Assessment (measuring and validating the biological and geochemical processes of bioremediation); and (6) Acceleration (developing effective methods for accelerating and optimizing bioremediation rates). University scientists continue to form the core of the NABIR science team that networks with the broader academic community as well as with scientists at the National Laboratories and at other agencies.

The NABIR Field Research Center (FRC) at Oak Ridge is characterizing the subsurface water flow and contaminant transport, and modeling subsurface flow, transport, and biogeochemistry at the FRC. Initial results will be published in FY 2002 and will help determine the efficacy of removing nitrate and injecting electron donors to precipitate and, therefore, immobilize uranium. The NABIR program will take advantage of the newly completed genomic sequence of three important metal and radionuclide-reducing microorganisms to study the regulation and expression of genes that are important in bioremediation. Knowledge of the regulation of genes involved in metal-reduction, such as the cytochromes, will determine the effect of co-contaminants, such as nitrate or other metals and radionuclides on the ability of microorganisms to immobilize the metals and radionuclides. Researchers working on *Geobacter sulfurreducens*, *Desulfovibrio vulgaris*, and *Shewanella oneidensis* will be able to use the genetic sequence and laboratory techniques such as micro-arrays to determine the enzymatic pathways for the reduction of uranium.

In FY 2003, research will focus on the completion of two critical field experiments at the NABIR FRC near the Y-12 area at the Oak Ridge Reservation. The first experiment will use "push-pull" technology to probe the structure and function of undisturbed microbial communities in the subsurface contaminated with uranium and nitrate. This will be the first time this new technology has been tested in a radionuclide-contaminated site. The second experiment will provide valuable information on the use of bioremediation to remove uranium from groundwater in which nitrate is a co-contaminant--a common problem at DOE sites.

**Performance will be measured:** By the end of FY 2003, the program will demonstrate whether certain nutrient additions stimulate subsurface microorganisms to immobilize uranium, thereby reducing its concentration and transport in soil water and groundwater. The demonstration will be in a contaminated subsurface environment where the co-contaminant nitrate is also present and will confirm the potential of biotechnology for environmental remediation of radionuclides.

**Performance will also be measured** by the successful demonstration, in partnership with EM-50, of the reliability of using new biologically based technologies for monitoring radionuclide contaminants and the microbial communities that can bioremediate those contaminants. These include antibody-based sensors for detecting uranium and certain metals, as well as nucleic acid based technologies for assessing the structure and functioning of microbial communities in contaminated environments.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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■ **General Plant Projects (GPP)** ..... **4,800**     **4,791**     **4,811**

The General Plant Projects (GPP) funding is for minor new construction, other capital alterations and additions, and for buildings and utility systems such as replacing piping in 30 to 40-year old buildings, modifying and replacing roofs, and HVAC upgrades and replacements. Funding of this type is essential for maintaining the productivity and usefulness of Department-owned facilities and in meeting its requirement for safe and reliable facilities operation. This subprogram includes landlord GPP funding for Pacific Northwest National Laboratory (PNNL) and for Oak Ridge Institute for Science and Education (ORISE). The total estimated cost of each GPP project will not exceed \$5,000,000.

The effort will continue rehabilitation and upgrade of research facilities in the 300 area of the PNNL, including beginning the replacement of sanitary water piping in a 40 year old building used for research, refurbishing 20-year old laboratory space, and reconfiguring space in a 45 year old building to better accommodate current scientific research projects.

■ **General Purpose Equipment (GPE)** ..... **1,167**     **1,164**     **1,169**

The General Purpose Equipment (GPE) funding will continue to provide general purpose equipment for PNNL and ORISE such as updated radiation detection monitors, information system computers and networks, and instrumentation that supports multi-purpose research.

**Clean Up Research** ..... **45,449**     **47,502**     **38,190**

■ **Clean Up Research** ..... **1,502**     **2,452**     **2,463**

The modest program in clean up research will characterize the geologic, chemical, and physical properties that affect the rate and effectiveness of a variety of environmental remediation and waste-stream cleanup methods, including bioremediation.

Research will support laboratory and field studies at universities and DOE laboratories to identify and characterize the biophysical and chemical properties of environmental pollutants in contaminated environments and waste streams, especially how those properties influence the efficacy of various remediation and waste-stream cleanup methods. In FY 2003, research in in-situ approaches is continued on challenging problems of mixed wastes containing complex mixtures of organic wastes, metals, and radionuclides.

Much of this research will be conducted in collaboration with the Office of Environmental Management (EM).

■ **Environmental Management Science Program** ..... **36,067**     **37,050**     **29,886**

The goal of the Environmental Management Science Program (EMSP), transferred in FY 2003 from EM to the BER program, is to support basic research that improves the science base underpinning the clean up of DOE sites. Traditional clean up strategies may not work or be cost effective for many of the challenges that threaten the successful closure of DOE sites. The EMSP, through its support of basic research aims to develop and validate technical solutions to complex problems,



(dollars in thousands)

FY 2001	FY 2002	FY 2003
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provide innovative technical solutions where there are none, and lead to future risk reduction and cost and time savings. The goal of the EMSP is to support basic research projects that could lead to specific demonstration projects and new clean up strategies. It is the intent or the expectation of the EMSP that the basic research projects funded offer the potential of having specific practical applications or specific timelines for the development of applications for waste cleanup.

Basic research that addresses the broad technical and scientific uncertainties associated with DOE site clean up will continue to be funded through a process of competitive peer review. The most scientifically meritorious research proposals and applications will be funded based on availability of funds and programmatic relevance to ensure a complete and balanced research portfolio that addresses DOE needs. The Office of Environmental Management will be consulted. Research will be funded at universities, national laboratories, and at private research institutes and industries.

■ **Savannah River Ecology Laboratory** ..... **7,880**      **8,000**      **5,841**

This activity supports, through a cooperative agreement with the University of Georgia, a long-term (40+ years) ecological research activity aimed at reducing the cost of clean up and remediation while ensuring biodiversity at the restored environment. Peer-reviewed research will be supported to understand contaminant behavior in the environment, to elucidate molecular mechanisms of toxicity from environmental contaminants, to develop cheaper and more environmentally sound remediation approaches, and to assess the ecological risks of environmental contaminants. Characterizing and understanding the impacts of environmental contamination on intact, living ecosystems is a complex and long-term process since the research is dependent on natural cycles of growth, reproduction, and normal environmental variation. A sustained investment is required to understand the complex interactions of ecosystems with environmental contaminants.

**Facility Operations: William R. Wiley Environmental Molecular Sciences Laboratory (EMSL)** ..... **31,248**      **37,333**      **37,948**

■ **Operating Expenses**..... **26,798**      **34,339**      **35,959**

The EMSL is a scientific user facility focused on conducting interdisciplinary, collaborative research in molecular-level environmental science. Operating funds are essential to allow the EMSL to operate as a user facility, and are used for maintenance of buildings and instruments, utilities, staff support for users, environment, safety and health compliance activities, and communications. With over 100 leading-edge instruments and computer systems, the EMSL annually supports approximately 1000 users. University scientists form the core of the EMSL science team that networks with the broader academic community as well as with scientists at other agencies. EMSL users have access to unique instrumentation for environmental research, including the 512-processor, high performance computer system, a suite of nuclear magnetic resonance spectrometers ranging from 300 MHz to 900 MHz, a suite of mass spectrometers, including an 11.5 Tesla high performance mass spectrometer, laser desorption and ablation instrumentation, ultra-high vacuum scanning tunneling and atomic force microscopes, and controlled atmosphere environmental chambers.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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The new 3-4 Teraflop high performance computer is being used for model code development in molecular geochemistry and biogeochemistry, and numerical modeling of reactive transport in the subsurface, chemical processing and catalysis, aerosol formation and chemical transformations and climate modeling and simulation. The computer also assists the EMSL focus on structural genomics.

**Performance will be measured** by (1) initiating operation of a new high performance computer at the EMSL and (2) having unscheduled operational downtime on EMSL instrumentation and computational resources not to exceed 10 percent.

- **Capital Equipment** ..... **4,450**      **2,994**      **1,989**

Capital equipment support for the EMSL enables instrument modifications needed by collaborators and external users of the facility as well as the purchase of state-of-the-art instrumentation to keep EMSL capabilities at the leading edge of molecular-level scientific research. Increased capital equipment funding (\$3,000,000) in FY 2001 supported the upgrade of user capabilities through the acquisition of additional mass spectrometers and Nuclear Magnetic Resonance (NMR) spectrometers for structural biology research.

- SBIR/STTR** ..... **0**      **1,569**      **2,692**

In FY 2001 \$1,242,000 and \$74,000 were transferred to the SBIR and STTR programs, respectively. FY 2002 and FY 2003 amounts are estimated requirements for the continuation of these programs.

- Total, Environmental Remediation** ..... **104,235**      **114,401**      **109,530**

### Explanation of Funding Changes from FY 2002 to FY 2003

FY 2003 vs. FY 2002 (\$000)
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#### Bioremediation Research

- Increased support for bioremediation research to expand research on microbially-mediated transformations of metals and radionuclides and how these processes can be altered to immobilize contaminants in place in subsurface environments. .... +2,678
- General Plant Projects continued at near FY 2002 level..... +20
- General Purpose Equipment continued at near FY 2002 level. .... +5
- Total, Bioremediation Research ..... +2,703

FY 2003 vs. FY 2002 (\$000)
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**Clean Up Research**

■ Clean Up Research continued at near FY 2002 level. ....	+11
■ Environmental Management Science program transferred in FY 2003 from the Office of Environmental Management to the BER program continued at a reduced level. ....	-7,164
■ Savannah River Ecology Laboratory transferred in FY 2003 from the Office of Environmental Management to the BER program continued at a reduced level. ....	-2,159
Total, Clean Up Research.....	-9,312

**Facility Operations**

■ EMSL funding increase provides for additional user support. ....	+615
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**SBIR/STTR**

■ SBIR/STTR increases due to increase in research funding for the Environmental Remediation program. ....	+1,123
Total Funding Change, Environmental Remediation.....	-4,871

# Medical Applications and Measurement Science

## Mission Supporting Goals and Objectives

The goal of the Medical Applications and Measurement Science subprogram is to deliver relevant scientific knowledge that will lead to innovative diagnostic and treatment technologies for human health. The research builds on unique DOE capabilities in physics, chemistry, engineering, and biology. Research will lead to new metabolic labels and imaging detectors for medical diagnosis; tailor-made radiopharmaceutical agents and beam delivery systems for treatment of inoperable cancers; and the ability to predict structure and behavior of cells and tissues to better engineer targeted drugs, biosensors, and medical implants. The basic research technologies growing out of this program offer applications for study, detection, diagnosis and early intervention of biochemical, bacterial, and viral health risks of biological, and/or gross environmental insults such as bioterrorism.

The modern era of nuclear medicine is an outgrowth of the original charge of the Atomic Energy Commission (AEC), "to exploit nuclear energy to promote human health." From the production of a few medically important radioisotopes in 1947, to the development of production methods for radiopharmaceuticals used in standard diagnostic tests in millions of patients throughout the world, to the development of ultra-sensitive diagnostic instruments, e.g. the PET (positron emission tomography) scanner, the medical applications program has led and continues to lead the field of nuclear medicine.

Today the program seeks to develop new applications of radiotracers in diagnosis and treatment in light of the latest concepts and developments in genomic sciences, structural and molecular biology, computational biology and instrumentation. Using non-invasive technologies and highly specific radiopharmaceuticals, BER is ushering in a new era of brain mapping, and highly specific disease diagnostics. New tools will enable the real-time imaging of gene expression in a developing organism.

Research capitalizes on the National Laboratories' unique resources and expertise in biological, chemical, physical, and computational sciences for technological advances related to human health. The National Laboratories have highly sophisticated instrumentation (neutron and light sources, mass spectroscopy, high field magnets), lasers and supercomputers, to name a few, that directly impact research on human health. Research is directed to fundamental studies in medical imaging, biological and chemical sensors, laser medicine and informatics. This research is highly complementary to and coordinated with clinical research at the National Institutes of Health (NIH) and to basic research in the NIH intramural and extramural programs.

Measurement Science research emphasizes new sensor instrumentation for cleanup efforts and new imaging instrumentation having broad application in the life and medical sciences.

The Medical Applications and the Measurement Science subprogram continues a substantial involvement of academic scientists along with the scientists in the National Laboratories.

## Funding Schedule

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
Medical Applications .....	87,276	113,825	38,701	-75,124	-66.0%
Measurement Science .....	5,911	5,935	5,961	+26	+0.4%
SBIR/STTR .....	0	3,239	1,186	-2,053	-63.4%
<b>Total, Medical Applications and Measurement Science .....</b>	<b>93,187</b>	<b>122,999</b>	<b>45,848</b>	<b>-77,151</b>	<b>-62.7%</b>

## Detailed Program Justification

(dollars in thousands)

	FY 2001	FY 2002	FY 2003
<b>Medical Applications.....</b>	<b>87,276</b>	<b>113,825</b>	<b>38,701</b>
<ul style="list-style-type: none"> <li> <span style="display: inline-block; width: 1em; height: 1em; background-color: black; margin-right: 0.5em;"></span> <b>Boron Neutron Capture Therapy (BNCT) and novel cell-directed cancer therapies .....</b> </li> </ul>	<b>10,082</b>	<b>9,941</b>	<b>4,870</b>

In FY 2003, funding for the followup of all patients treated in the human clinical trials of boron neutron capture therapy (BNCT) at Brookhaven National Laboratory and the Massachusetts Institute of Technology will be completed with the transfer of clinical technology to the National Cancer Institute. The basic drug development research for BNCT will evolve into a new program of innovative approaches to cell-targeted ablation therapy for cancer with in-vivo radiation techniques. Success of the program will depend on key partnerships with scientists from the National Laboratories and academia. The emphasis of this program will be on the therapeutic use of ionizing radiation that may be achieved with radionuclide therapy and novel methods of tumor targeting. The specific goals include the development of novel therapeutic agents and delivery techniques to target and treat cancer at the cellular level. Research will address such complex challenges as chemical ligand synthesis, tumor-targeting, and dosimetry.

Overall program objectives include: (1) techniques to ensure highly selective tumor-targeting by the proposed therapeutic agents; (2) efficient screening techniques for selecting candidate therapeutic agents for in-vivo testing; (3) research suggesting a reasonable likelihood of success for in-vivo targeting of primary tumors and their metastases in pre-clinical animal trials; (4) reliable approaches for dosimetry calculations to normal tissues and to tumor sites based on 3-dimensional modeling; (5) measurement techniques for accurately assessing the success of tumor-targeting in vivo; and (6) measurement techniques for assessing therapy effects in vivo at the molecular, cellular and metabolic levels.

**Performance will be measured** by the number of tumor therapeutic agents that perform sufficiently well in pre-clinical evaluations over five years to deserve consideration for clinical trials by NIH and/or private industry.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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**Performance will be measured:** By the end of FY 2003, all the boron neutron capture therapy (BNCT) clinical trials will be completed with clinical data collection, and transfer of the clinical data to the National Cancer Institute as the foundation for an advanced treatment modality for cancer.

■ **Radiopharmaceutical Design and Synthesis** ..... 26,065 24,340 24,445

BER will support research on radiopharmaceutical design and synthesis using concepts from genomics as well as computational biology and structural biology. BER will continue research into radiolabeling of monoclonal antibodies for cancer diagnosis and new radiotracers for the study of brain and heart function. Molecules directing or affected by homeostatic controls always interact and, thus, are targets for specific molecular substrates. The substrate molecules can be tailored to fulfill a specific need and labeled with appropriate radioisotopes to become measurable in real time in the body on their way to, and during interaction with their targets, allowing the analysis of molecular functions in the homeostatic control in health and disease. The function of radiopharmaceuticals at various sites in the body is imaged by nuclear medical instruments, such as, gamma ray cameras and positron emission tomographs (PET). This type of imaging refines diagnostic differentiation between health and disease at the molecular/metabolic levels as well as often leading to more effective therapy. If labeled with high energy-emitting radioisotopes, the substrate molecules, carrying the radiation dose may be powerful tools for targeted molecular therapy especially of cancer.

BER will also develop nuclear medicine driven technologies to image mRNA transcripts in real time in tissue culture and whole animals. Currently the expression of endogenous genes in animals (including humans) cannot be imaged, at least not directly. However, given the astounding pace of biotechnology development, such imaging is an attainable goal. This research includes an emphasis on nucleic acid biochemistry, radioactive ligand synthesis and macromolecular interactions. It addresses the functional consequences of gene expression by targeting and perturbing the activity of a particular gene in living cells or animals. It also develops new biological applications using optical and radionuclide imaging devices for imaging specific gene expression in real time in both animals and humans. Methods such as combinatorial chemistry techniques will be used to develop antisense radiopharmaceuticals that hybridize DNA probes to RNA transcripts in highly specific ways to block their activity or function. Molecular signal amplification methods that work in vivo at the mRNA level will be developed. Drug-targeting technology will be developed to such an extent that the various biological barriers can be safely surmounted in vivo. The research will evaluate the clinical potential of real-time imaging of genes at work in cells, tissues, and whole organisms, including humans. This information will have applications ranging from understanding the development of a disease to the efficacy of treatments for the disease. This new technology will strongly impact developmental biology, genome research, and medical sciences.

**Performance will be measured:** By the end of FY 2003, through radiopharmaceutical and molecular nuclear medicine research, three positron emission tomography (PET) radiotracers with precise cellular, subcellular, and molecular targeting capability will be developed as potential imaging agents for nuclear medicine research and clinical use to study brain disorders due to substance abuse and

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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mental illnesses (such as Alzheimer's and Parkinson's diseases), cancer diagnosis and treatment, heart-function-related ailments, therapeutic gene expression in the whole animals, and for monitoring progress to therapy.

■ **Multimodal Imaging Systems and Medical Photonics..... 10,004 9,753 9,386**

In FY 2003, BER will emphasize support in multimodal imaging systems for study of human brain function and continue to explore the combination of nuclear medicine imaging systems with magnetic resonance imaging. The research will continue to develop innovative imaging instrumentation and will transfer the relevant technology into clinical medicine. PET and MRI instrumentation systems will be developed to image small animals with high resolution. The program will continue to support research in brain imaging including substance abuse, mental illness, Parkinson's disease, Alzheimer's disease, and studies of neurochemical metabolism.

**Performance will be measured:** By the end of FY 2003, 1-3 advanced radiotracer imaging camera devices, that approach the fundamental limits of spatial resolution and detector sensitivity, will be available to detect breast cancer to differentiate benign as compared to malignant growth, and will measure biological function in small animals as the models of human disease.

BER will also expand its research program at the National Laboratories by capitalizing on their unique resources and expertise in the biological, physical, chemical, and computational, sciences to develop new research opportunities for technological advancement related to human health. Due to the medical nature of the program, all research activities are joint activities between the National Laboratories and medical research centers. The program emphasizes biomedical imaging, novel sensing devices, spectroscopy, and related informatics systems. It will advance fundamental concepts, create knowledge from the molecular to the organ systems level, and develop innovative processes, instruments, and informatics systems to be used for the prevention, diagnosis, and treatment of disease and for improving health care in the Nation. Emphasis is placed on:

*Biomedical Imaging* – is the development of novel medical imaging systems. BER will combine optical imaging with other traditional medical imaging systems such as MRI, PET, and SPECT (single photon emission computed tomography) and will develop small imaging systems that image in real-time under natural physiological conditions. A major objective is improving the reliability and cost-effectiveness of medical imaging technologies. Technology and detector systems will be developed to capitalize on recent findings of the human genome project that will enable imaging of gene expression in real time that will have a critical impact on biomedical research and medical diagnosis. The BER program has played a leading role in the development of new positron emission tomography (PET) instrumentation as well as new chemistries for applying PET to diagnosis of cancer and other diseases. A high priority is placed on transfer of the new PET technologies into clinical research and practice.

*Medical Photonics* – is the development of advanced optical systems, including lasers, that will enhance the monitoring, detection, and treatment of disease. BER will expand its development of an artificial retina that can convert light signals into physiological electrical impulses.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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*Smart Medical Instrumentation* – is the development and fabrication of “smart” medical instruments that can operate within the body either remotely or independently to monitor, detect, and treat various medical dysfunctions. This includes the development and fabrication of biological sensors that can be used to detect or monitor various physiological functions and disease in the body in real-time.

The ultimate goal of the program is to support basic research and technology development that will ultimately lead to the development of technology that can be transferred to the National Institutes of Health for clinical testing or to industry for further commercial development. This research takes advantage of unique resources at DOE facilities and is highly complementary to and coordinated with clinical research at the National Institutes of Health (NIH) and to basic research in the NIH intramural and extramural programs.

**Performance will be measured** by the enhancement of micro-PET and micro-CT scanners so that these unique and powerful tools can be used to enhance basic biomedical research in medical centers, leading to improved human health care, and over the next five years, mutually beneficial research partnerships between the BER Advanced Medical Technology Program and the Intramural Clinical Research Programs at the National Institutes of Health (NIH) will deliver two new biosensor and infrared thermography technologies using the physical science expertise of the DOE national laboratories. The technologies will aid in the detection of disease at an early stage.

- **Congressional Direction**..... **41,125**    **69,791**    **0**

Congressional direction in FY 2001 for School of Public Health, University of South Carolina; Nuclear Medicine and Cancer Research Capital Program, University of Missouri-Columbia; Discovery Science Center in Orange County, California; Children’s Hospital Emergency Power Plant in San Diego; Center for Science and Education at the University of San Diego; Bone Marrow Transplant Program at Children’s Hospital Medical Center Foundation in Oakland, CA; North Shore Long Island Jewish Health System, New York; Museum of Science and Industry, Chicago; Livingston Digital Millenium Center, Tulane University; Center for Nuclear Magnetic Resonance, University of Alabama-Birmingham; Nanotechnology Engineering Center at the University of Notre Dame of South Bend, Indiana; National Center for Musculoskeletal Research, Hospital for Special Surgery, New York; High Temperature Super Conducting Research and Development, Boston College; Positron Emission Tomography Facility, West Virginia University; Advanced Medical Imaging Center, Hampton University; Child Health Institute of New Brunswick, New Jersey; Linear Accelerator for University Medical Center of Southern Nevada; Medical University of South Carolina Oncology Center; National Foundation for Brain Imaging; Science and Technology Facility at New Mexico Highlands University; and Inland Northwest Natural Resources Research Center at Gonzaga University.



(dollars in thousands)

FY 2001	FY 2002	FY 2003
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Congressional direction in FY 2002 for Positron Emission Tomography Center at the University of South Alabama; Gulf Coast Cancer Center and Research Institute for Nuclear Magnetic Resonance Imaging at the University of Alabama Birmingham; University of South Alabama research, in cooperation with industry and the Cooperative Research Network of the National Rural Electric Cooperative Association, on a fuel cell powered home using the Smart Energy Management Control System; Library and Regional Resource Learning Center at Spring Hill College; South Alabama Medical Education Outreach Program; University of Florida Genetics Institute; Linear Accelerator for the Baystate Medical Center; Cancer Institute at New Jersey; Institute for Molecular Biosciences at the University of Arizona; Stanley Scott Cancer Center at Louisiana State University; Infotonics Center of Excellence in Rochester New York; Joint Collaboration on Advanced Nanotechnology and Sensors with the University of New Orleans, Louisiana State University, and Louisiana Tech; Breast Cancer Program at the North Shore-Long Island Jewish Health System; Functional Magnetic Resonance Imaging Machine at the University of Texas at Dallas and the University of Texas Southwestern Medical Center's Center for Brain, Cognition, and Behavior; Integrated Environmental Research and Services Program at Alabama A&M University; Energy Efficiency Initiative at the Carolinas Health Care System; Multidisciplinary Research Facility at the College of Engineering, University of Notre Dame; Linear Accelerator for the Burbank Regional Cancer Center in Fitchburg, Massachusetts; Hampshire College's National Center for Science Education; Audubon Biomedical Science and Technology Park at Columbia University; McFadden Science Center at Texas Wesleyan University; Emergency Power Supply System at Cedars-Sinai Medical Center; Rush-Presbyterian-St. Luke's Medical Center; Nanoscience Facility at Purdue University; Julie and Ben Rogers Cancer Institute; School of Public Health at the University of South Carolina; Continued Development of the Life Science Building at Brown University; Environmental Modeling at the University of North Carolina at Chapel Hill; Renovation of the Science, Technology, and Engineering Research Complex at Jackson State University; PowerGrid Simulator at Drexel University and the New Jersey Institute of Technology; Positron Emission Tomography Facility at West Virginia University; Linear Accelerator for the University Medical Center of Southern Nevada; Research Foundation of the University of Nevada-Las Vegas; University of Nevada-Las Vegas for Continued Study of the Biological Effects of Exposure to Low-level Radioactivity; Biomolecular Nuclear Magnetic Resonance Instrument at the Medical University of South Carolina; Oncology Center of the Medical University of South Carolina; National Center of Excellence in Photonics and Microsystems in New York; Institute of Comparative Genomics at the American Museum of Natural History; Inland Northwest Natural Resources Center at Gonzaga University; Hall of Paleontology at the Field Museum; Center for Catalysis at Iowa State University; Human Genome Project at the University of Southern California; Biomedical Research at Creighton University; Child Health Institute of New Brunswick, New Jersey; Oregon Renewable Energy Center; Superconductor Research at Boston College; Natural Renewable Energy Laboratory in Hawaii; Rochester Institute of Technology Microelectronics Technology Program; Operations and Capital Investment at the Mental Illness and Neuroscience Discovery Institute; and University of Missouri-Columbia to Expand the Federal Investment in the University's Nuclear Medicine and Cancer Research Capital Program.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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**Measurement Science**..... **5,911**      **5,935**      **5,961**

BER will continue research on new sensor instrumentation for characterizing the chemical composition of contaminated subsurface environments in support of the Department’s environmental cleanup efforts of highly radioactive chemical wastes.

The research will include the development of new environmental sensors that are better, faster, and more economical than existing laboratory techniques. New field-based sensors that take advantage of novel biotechnologies will be ready for deployment. The new sensors will include antibody and nucleic acid approaches that have precedence in other applications but will be new to bioremediation at DOE legacy sites.

Research into new imaging instrumentation for life sciences and biomedical sensor applications will be continued. Capital equipment funds will be used for research to develop new instrumentation having broad application in the life and medical sciences. BER will continue research on medical applications of laser technology at the National Laboratories and at universities.

**SBIR/STTR**..... **0**      **3,239**      **1,186**

In FY 2001 \$2,357,000 and \$143,000 were transferred to the SBIR and STTR programs, respectively. FY 2002 and FY 2003 amounts are estimated requirements for the continuation of these programs.

**Total, Medical Applications and Measurement Science** ..... **93,187**      **122,999**      **45,848**

### Explanation of Funding Changes from FY 2002 to FY 2003

FY 2003 vs. FY 2002 (\$000)
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#### Medical Applications

- Boron Neutron Therapy (BNCT) program is completed and research on novel cell-directed cancer therapies is initiated ..... -5,071
- Radiopharmaceutical Design and Synthesis and Multimodal Imaging Systems and Medical Photonics are continued at near FY 2002 levels. .... -262
- Decrease due to Congressional direction in FY 2002. .... -69,791

Total Funding Change, Medical Applications..... -75,124

#### Measurement Science

- Measurement Science will continue at near FY 2002 levels..... +26

FY 2003 vs. FY 2002 (\$000)
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**SBIR/STTR**

<ul style="list-style-type: none"> <li>■ SBIR/STTR decreases due to decrease in research funding for the Medical Applications and Measurement Science program.....</li> </ul>	<u>-2,053</u>
Total Funding Change, Medical Applications and Measurement Science.....	<u><u>-77,151</u></u>

# Construction

## Mission Supporting Goals and Objectives

Construction is needed to support the research under the Biological and Environmental Research Program (BER) program. Cutting-edge basic research requires that state-of-the-art facilities be built or existing facilities modified to meet unique BER requirements.

### Funding Schedule

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
Construction .....	2,495	11,405	0	-11,405	--

### Detailed Program Justification

(dollars in thousands)

	FY 2001	FY 2002	FY 2003
<b>Construction</b> .....	<b>2,495</b>	<b>11,405</b>	<b>0</b>

- The Laboratory for Comparative and Functional Genomics at Oak Ridge National Laboratory will provide a modern gene function research facility to help understand the function of newly discovered human genes, to support DOE research programs and to provide protection for the genetic mutant mouse lines created during the past 50 years. This new facility will replace a 50-year old animal facility with rapidly escalating maintenance costs still in use at Oak Ridge.

**Performance will be measured:** By the end of FY 2003, construction of the Center for Comparative and Functional Genomics at Oak Ridge National Laboratory will be completed on schedule.

### Explanation of Funding Changes from FY 2002 to FY 2003

	FY 2003 vs. FY 2002 (\$000)
<b>Construction</b>	
<ul style="list-style-type: none"> <li> <span style="display: inline-block; width: 1em; height: 1em; background-color: black; margin-right: 0.5em;"></span>           Full funding for the construction of the Laboratory for Comparative and Functional Genomics provided in FY 2002. ....         </li> </ul>	-11,405

# Capital Operating Expenses & Construction Summary

## Capital Operating Expenses

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
General Plant Projects .....	8,094	4,791	4,811	+20	+0.4%
Capital Equipment.....	44,538	17,543	17,047	-496	-2.8%
<b>Total Capital Operating Expenses.....</b>	<b>52,632</b>	<b>22,334</b>	<b>21,858</b>	<b>-476</b>	<b>-2.1%</b>

## Construction Projects

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Appropriations	FY 2001	FY 2002	FY 2003	Unappropriated Balance
01-E-300, Laboratory for Comparative and Functional Genomics, ORNL.....	13,900	0	2,495	11,405	0	0
<b>Total, Construction .....</b>		<b>0</b>	<b>2,495</b>	<b>11,405</b>	<b>0</b>	<b>0</b>

## Major Items of Equipment (TEC \$2 million or greater)

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Appropriations	FY 2001	FY 2002	FY 2003	Acceptance Date
DNA Repair Protein Complex Beamline, ALS.....	4,490	0	4,490	0	0	FY 2001
<b>Total, Major Items of Equipment ....</b>		<b>0</b>	<b>4,490</b>	<b>0</b>	<b>0</b>	

# Basic Energy Sciences

## Program Mission

Basic Energy Sciences (BES) and its predecessor organizations have supported a program of fundamental research focused on critical mission needs of the Nation for over five decades. The federal program that became BES began with the research effort that was initiated to help defend our Nation during World War II. The diversified program was organized into the Division of Research with the establishment of the Atomic Energy Commission in 1946 and was later renamed Basic Energy Sciences as it continued to grow through legislation included in the Atomic Energy Act of 1954, the Energy Reorganization Act of 1974, the Department of Energy Organization Act of 1977, and the Energy Policy Act of 1992.

Today, the mission of the BES program – a multipurpose, scientific research effort – is to foster and support fundamental research in focused areas of the natural sciences in order to expand the scientific foundations for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use. BES delivers the knowledge needed to support the President's National Energy Plan for improving the quality of life for all Americans. In addition, BES works cooperatively with other agencies and the programs of the National Nuclear Security Administration to discover knowledge and develop tools to strengthen national security and combat terrorism. As part of its mission, the BES program plans, constructs, and operates major scientific user facilities to serve researchers at universities, national laboratories, and industrial laboratories.

## Strategic Objectives

- SC4:** Provide leading scientific research programs in materials sciences and engineering, chemical sciences, biosciences, and geosciences that underpin DOE missions and spur major advances in national security, environmental quality, and the production of safe, secure, efficient, and environmentally responsible systems of energy supply; as part of these programs, by 2010, establish a suite of Nanoscale Science Research Centers and a robust nanoscience research program, allowing the atom-by-atom design of revolutionary new materials for DOE mission applications, and restoring U.S. preeminence in neutron scattering research and facilities.
- SC7:** Provide major advanced scientific user facilities where scientific excellence is validated by external review; average operational downtime does not exceed 10% of schedule; construction and upgrades are within 10% of schedule and budget; and facility technology research and development programs meet their goals.

Progress toward accomplishing these Strategic Objectives will be measured by Program Strategic Performance Goals, Indicators, and Annual Targets, as follows:

## Program Strategic Performance Goals

**SC4-1:** Build leading research programs in the scientific disciplines encompassed by the BES mission areas and provide world-class, peer-reviewed research results cognizant of DOE needs as well as the needs of the broad scientific community (Materials Sciences and Engineering Subprogram; Chemical Sciences, Geosciences, and Energy Biosciences Subprogram).

### Performance Indicator

Validation of results by merit review with external peer evaluation.

### Performance Standards

As discussed in Office of Science Corporate Context/Executive Summary.

## Annual Performance Results and Targets

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
<p>BES used expert advisory committees and rigorous peer review committees to ascertain that the research performed by investigators in universities and DOE laboratories was focused and outstanding. An additional indicator of the success of our scientific research was the recognition through the awards received by our researchers and by the broader scientific community. (SC4-1) [Met Goal]</p>	<p>Competitively select and peer review at least 80 percent of all new research projects, and evaluate approximately 30 percent of ongoing projects using guidelines defined in 10 CFR 605 for the university projects and similar guidelines established by BES for the laboratory projects. (SC4-1)</p>	<p>Competitively select and peer review at least 80 percent of all new research projects, and evaluate approximately 30 percent of ongoing projects using guidelines defined in 10 CFR 605 for the university projects and similar guidelines established by BES for the laboratory projects. (SC4-1)</p>
	<p>As part of the continuing, high-level review of the management processes and the quality, the relevance, and the national and international leadership of BES programs, review the chemical sciences activities using a BESAC-chartered Committee of Visitors. In addition, evaluate the following ongoing efforts using BESAC- and BES-sponsored workshops with the goal of directing the activities toward international leadership and relevance to emerging technologies: superconductivity. Publish results and continue to structure BES programs per results. (SC4-1)</p>	<p>As part of the continuing, high-level review of the management processes and the quality, the relevance, and the national and international leadership of BES programs, review the materials sciences and engineering activities using a BESAC-chartered Committee of Visitors. In addition, evaluate the following ongoing efforts using BESAC- and BES-sponsored workshops with the goal of directing the activities toward international leadership and relevance to emerging technologies: photovoltaics, radiation effects, materials synthesis and processing, and catalysis. Publish results and continue to structure BES programs per results. (SC4-1)</p>

**SC4-2:** Enable U.S. leadership in nanoscale science, allowing the atom-by-atom design of materials and integrated systems of nanostructured components having new and improved properties for applications as diverse as high-efficiency solar cells and better catalysts for the production of fuels (Materials Sciences and Engineering subprogram; Chemical Sciences, Geosciences, and Energy Biosciences subprogram).

**Performance Indicator**

Validation of results by merit review with external peer evaluation.

**Performance Standards**

As discussed in Office of Science Corporate Context/Executive Summary.

**Annual Performance Results and Targets**

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
Initiated 76 grants to universities (from 417 grant applications) and 12 projects at DOE laboratories (from 46 Field Work Proposals) in selected areas of nanoscale science, engineering, and technology. (SC4-2) [Met Goal]	Begin engineering and design of three Nanoscale Science Research Centers. (SC4-2)	Begin construction of one Nanoscale Science Research Center meeting the cost and timetables within 10 percent of the baselines given in the construction project data sheets, project number 03-R-312. Conduct engineering and design activities to establish construction baselines on the two other Nanoscale Science Research Centers. (SC4-2)
	Initiate approximately 40 grants to universities and 6 projects at DOE laboratories in selected areas of nanoscale science, engineering, and technology. (SC4-2)	Establish the instrument suites and identify fabrication capabilities for the new Nanoscale Science Research Centers based upon user community input at national workshops held in late FY 2001 and FY 2002. (SC4-2)

**SC4-3:** Develop advanced research instruments for x-ray diffraction, scattering, and imaging to provide diverse communities of researchers with the tools necessary for exploration and discovery in materials sciences and engineering, chemistry, earth and geosciences, and biology (Materials Sciences and Engineering subprogram; Chemical Sciences, Geosciences, and Energy Biosciences subprogram).

**Performance Indicator**

Validation of results by merit review with external peer evaluation.

**Performance Standards**

As discussed in Office of Science Corporate Context/Executive Summary.



## Annual Performance Results and Targets

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
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Select and begin upgrade/fabrication of at least two instruments at the BES synchrotron light sources, based on peer review of submitted proposals, to keep the facilities at the forefront of science. Because the lifetime of an instrument is about 7-10 years, this addresses the need to renew instruments on a regular basis. (SC4-3)

Establish collaborative, national R&D programs for common needs at the BES synchrotron light sources, e.g., for detectors and other components. (SC4-3)

**SC7-4A:** Manage BES facility operations and construction to the highest standards of overall performance using merit evaluation with independent peer review. (Materials Sciences and Engineering subprogram; Chemical Sciences, Geosciences, and Energy Biosciences subprogram).

### Performance Indicator

Validation of results by merit review with external peer evaluation.

### Performance Standards

As discussed in Office of Science Corporate Context/Executive Summary.

## Annual Performance Results and Targets

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
-----------------	-----------------	-----------------

BES scientific user facilities were maintained and operated so that the unscheduled downtime on average is less than 10 percent of the total scheduled operating time. The cost and schedule milestones for upgrades and construction of scientific user facilities, including the construction of the Spallation Neutron Source were met. [Met Goal]

Maintain and operate the BES scientific user facilities so the unscheduled downtime on average is less than 10 percent of the total scheduled operating time. Maintain the cost and schedule milestones within 10 percent for upgrades and construction of scientific user facilities. (SC7-4A)

Maintain and operate the BES scientific user facilities so the unscheduled downtime on average is less than 10 percent of the total scheduled operating time. Maintain the cost and schedule milestones within 10 percent for upgrades and construction of scientific user facilities. (SC7-4A)

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
	Continue upgrades on the major components of the SPEAR 3 storage ring at the Stanford Synchrotron Radiation Laboratory (SSRL), maintaining cost and schedule within 10 percent of baselines. At the end of FY 2002, the upgrade of SPEAR 3 will be 70 percent complete. (SC7-4A)	Complete the upgrade of the SPEAR 3 storage ring at the Stanford Synchrotron Radiation Laboratory (SSRL), maintaining cost and schedule within 10 percent of baselines. (SC7-4A)

SC7-4B: Restore U.S. preeminence in neutron scattering research, instrumentation, and facilities to provide researchers with the tools necessary for the exploration and discovery of advanced materials (Materials Sciences and Engineering subprogram; Chemical Sciences, Geosciences, and Energy Biosciences subprogram).

**Performance Indicator**

Validation of results by merit review with external peer evaluation.

**Performance Standards**

As discussed in Office of Science Corporate Context/Executive Summary.

**Annual Performance Results and Targets**

FY 2001 Results	FY 2002 Targets	FY 2003 Targets
	<p>Continue construction of the Spallation Neutron Source (SNS), meeting the cost and timetables within 10 percent of the baselines in the construction project data sheet, project number 99-E-334. At the end of FY 2002, construction of the SNS will be 47 percent complete. (SC7-4B)</p> <p>Select and begin fabrication of one additional instrument for the SNS. (SC7-4B)</p>	<p>Continue construction of the Spallation Neutron Source (SNS) meeting the cost and timetables within 10 percent of the baselines given in the construction project data sheet, project number 99-E-334. At the end of FY 2003, construction of the SNS will be 61 percent complete. (SC7-4B)</p> <p>Select and begin fabrication of one additional instrument for the SNS. Select and begin upgrade/fabrication of one instrument each at the High Flux Isotope Reactor and the Manuel Lujan, Jr. Neutron Scattering Center. Commitment at the Lujan Center is conditional upon LANSCE demonstrating reliable operations as determined by a BESAC review conducted in FY 2003. (SC7-4B)</p>

## Significant Accomplishments and Program Shifts

The BES program continues as one of the Nation's largest sponsors of fundamental research in the natural sciences and is uniquely responsible for supporting research impacting energy resources, production, conversion, efficiency, and the mitigation of the adverse impacts of energy production and use. In FY 2001, the program funded research in more than 150 academic institutions located in 48 states and in 13 Department of Energy (DOE) laboratories located in 9 states. BES supports a large extramural research program, with approximately 40% of the program's research activities sited at academic institutions.

The *National Energy Policy* noted that the U.S. economy grew by 126% since 1973, but energy use increased by only 30%. Approximately one-half to two-thirds of the savings resulted from technological improvements in products and services that allow consumers to enjoy more energy services without commensurate increases in energy demand. At the heart of these improvements is fundamental research. During this 30-year period, the basic research supported by the BES program has touched virtually every aspect of energy resources, production, conversion, efficiency, and waste mitigation. The basic knowledge derived from fundamental research has resulted in a vast array of advances, including • high-energy and high-power lithium and lithium ion batteries and thin-film rechargeable microbatteries; • thermoacoustic refrigeration devices that cool without moving parts and without the use of freons; • compound semiconductors, leading to the world's highest efficiency photovoltaic solar cells; • catalysts for the production of new polymers (annually, a multibillion dollar industry) and for a host of other products and energy-efficient processes; • high-strength, lightweight magnets for sensors and for small motors used in power steering and other vehicle functions; • strong, ductile alloys for use in high-temperature applications; • toughened (i.e., nonbrittle) ceramics for use in hammers, high-speed cutting tools, engine turbines, and other applications requiring lightweight, high-temperature materials; • new steels, improved aluminum alloys, magnet materials, and other alloys; • polymer materials for rechargeable batteries, car bumpers, food wrappings, flat-panel displays, wear-resistant plastic parts, and polymer-coated particles in lubricating oils; • new commercial processes for ethanol production, pulp and paper manufacturing, and *in planta* production of oils built on foundations laid by the Energy Biosciences activities; • processes for extraction of radioactive and hazardous metal ions from solutions for nuclear fuel purification/reprocessing and for cleanup of radioactive wastes; • the atomic-level understanding of combustion processes as a result of the creation of the Combustion Research Facility, where basic, applied, and industrial research are collocated; and • a host of new instruments, e.g. instruments based on high-temperature superconductors — “superconducting quantum interference devices” or SQUIDs for short — that can sense the minute magnetic fields that emanate from the human brain and heart. These advances came by exploiting the results of basic research that sought answers to fundamental questions.

The BES program also supports world-class scientific user facilities, providing outstanding capabilities for imaging and characterizing materials of all kinds from metals, alloys, and ceramics to fragile biological specimens and crystals. The BES synchrotron radiation light sources, the neutron scattering facilities, and the electron beam characterization centers represent the largest and best collection of such facilities supported by a single organization in the world. Annually, 8,000 researchers from universities, national laboratories, and industrial laboratories perform experiments at these facilities. Spurred by results of past investments and by innovations in accelerator concepts, the BES program continues its pioneering role in the development of new generations of scientific research instruments and facilities.

## **FY 2001 Honors and Awards**

Each year, principal investigators funded by BES win dozens of major prizes and awards sponsored by professional societies and by others. In addition, many are elected to fellowship in organizations such as the National Academy of Sciences, the National Academy of Engineering, and the major scientific professional societies. Paramount among the honors are six Nobel Prizes awarded to BES principal investigators since the mid-1980s. Selected major prizes and awards for FY 2001 include:

*From Acta Metallurgica, Inc.* -- Acta Metallurgica Gold Medal

*From ASM International* -- the 2001 ASM International Gold Medal

*From R&D Magazine* -- R&D 100 Award for the invention of the MOLYCAST Furnace, an environmentally friendly system of new energy efficient heating elements.

*From the Alexander von Humboldt Foundation of Germany* -- the Humboldt Research Award

*From the American Association of Engineering Societies* -- the John Fritz Medal

*From the American Chemical Society* -- the Award in Chemistry of Materials; the Award in Colloid or Surface Chemistry; the Arthur C. Cope Scholar Award; the Arthur W. Adamson Award for Distinguished Service in the Advancement of Surface Chemistry; the Nobel Laureate Signature Award for Graduate Education in Chemistry; the Award for Creative Research in Homogeneous or Heterogeneous Catalysis

*From the American Institute of Chemical Engineers* -- the William H. Walker Award

*From the American Physical Society* -- the Irving Langmuir Prize in Chemical Physics; the Herbert P. Broida Prize

*From the American Vacuum Society* -- the Medard W. Welch Award; the John A. Thornton Award

*From the American Welding Society* -- four recipients of the William Spraragen Award

*From the Computing Research Association* -- an Honorable Mention in the Computing Research Association's Outstanding Undergraduate Award

*From the Electrochemical Society* -- the David C. Graham Award in Physical Electrochemistry

*From the German Society for Physical Chemistry* -- the Jost Memorial Award

*From the Iron and Steel Society* -- the Geoffrey Belton Award

*From the Japan Fine Ceramics Association* -- the 2001 International Prize

*From the Materials Research Society* -- the Materials Research Society Medal for 2001

*From the Metals, Minerals, and Materials Society* -- the Robert Lansing Hardy Award

*From the Samsung Foundation* -- the Ho-Am Prize for Science

Twelve principal investigators were elected to the National Academy of Sciences, and six were elected to the National Academy of Engineering. Fifteen principal investigators were advanced to fellowship in the American Physical Society; seven in the American Academy of Arts and Sciences; one in the American Ceramics Society; four in the Minerals, Metals, and Materials Society; and two in the John Simon Guggenheim Memorial Foundation.

## Selected FY 2001 Science Accomplishments

### Materials Sciences and Engineering

- *Micro-size Light Emitters for Solid State Lighting Applications.* Energy savings of tens of billions of dollars per year could be achieved by replacement of household 100-watt light bulbs by white light emitting diodes (LED) made by mixing LEDs emitting primary colors. However, improved LED efficiency is necessary before such replacement becomes feasible. New research has shown that interconnecting hundreds of micro-size LEDs to replace larger conventional LEDs can boost the overall emission efficiency by as much as 60 percent.
- *A New Method for Obtaining Crystal Structures Without Large Crystals.* High-resolution x-ray diffraction using polycrystalline samples (“powders”) rather than traditional single-crystal samples has advanced to the point where the structures of complex materials including oxides, zeolites, and small organic structures can be solved. Advantages of powder diffraction are that it is not affected by crystal fracture and polycrystalline samples can be formed over a much wider range of conditions than large single crystals. Recently, powder diffraction was demonstrated for large molecules, such as proteins, that were considered far too complex for powder diffraction experiments. In addition to the many important applications to materials sciences, this technique will also be useful in chemistry and biosciences.
- *NMR and MRI Outside the Magnet.* NMR (nuclear magnetic resonance) imaging and MRI (magnetic resonance imaging) have required large high-field magnets that impose extremely uniform magnetic fields upon the sample. In many circumstances, however, it is impractical or undesirable to place or rotate objects and subjects within the bore of such a large magnet. A new approach for the recovery of highly resolved NMR spectra and MRI images of samples in grossly non-uniform magnetic fields was recently demonstrated. The approach will be useful for the enhanced study of fluids contained in porous materials, such as deep underground oil-well logging studies, and is expected to have dramatic research applications in chemistry, materials sciences, and biomedicine.
- *Terabit Arrays (One trillion bits per square inch).* A 300-fold increase in magnetic storage density has been achieved using a patented technique of self-assembly of block copolymers under the influence of a small voltage. The new technique is simple, robust, and extremely versatile. The key to this discovery lay in directing the orientation of nanoscopic, cylindrical domains in thin films of block copolymers. By coupling this with routine lithographic processes, large area arrays of nanopores can be easily produced. Electrochemical deposition of metals, such as cobalt and iron, produces nanowires that exhibit excellent magnetic properties, key to ultrahigh density magnetic storage. The nanowires are also being used as field emission devices for displays.
- *Observations of Atomic Imperfections.* A new electron beam technique has been developed that has measured atomic displacements to a record accuracy of one-hundredth of the diameter of an atom. Such small imperfections in atomic packing often determine the properties and behavior of materials, particularly in nano-structured devices. This capability has been made possible by a new technique that couples electron diffraction with imaging technology. The result is a greatly enhanced capability to map imperfections and their resulting strain fields in materials ranging from superconductors to multi-layer semiconductor devices.

- *Semiconductor Nanocrystals as “Artificial Leaves.”* Recent experiments demonstrated that carbon dioxide could be removed from the atmosphere with semiconductor nanocrystals. These “artificial leaves” could potentially convert carbon dioxide into useful organic molecules with major environmental benefits. However, to be practical, the efficiency must be substantially improved. New theoretical studies have unraveled the detailed mechanisms involved and identified the key factors limiting efficiency. Based on this new understanding, alternative means for improving efficiency were suggested that could lead to effective implementation of artificial leaves to alleviate global warming and the depletion of fossil fuels.
- *“Magic” Values for Nanofilm Thickness.* A key issue for nanotechnology is the structural stability of thin films and the devices made from nanostructures. It was recently demonstrated that nanofilms are significantly more stable at a few specific values of film thickness. The origin of this effect arises from the confinement of electrons within the film leading to electronic states with discrete energy values, much as atomic electrons are bound to the nucleus at discrete energy levels. Calculations demonstrated that increased stability occurred when the number of electrons present in the film completely filled the set of available states, just as filled electronic shells make the noble gases very stable.
- *Materials Resistant to Damage from Nuclear Waste.* The ability to predict the composition and structure of materials that are resistant to radiation damage, such as in nuclear waste storage, has been formulated on a firm scientific basis. Current nuclear waste storage materials cannot resist radiation damage for the required thousands of years because radioactive emissions in a storage material jostle atoms out of their carefully ordered arrangements. These materials become unstable and eventually leach into the environment. Computer simulations and experiments revealed that a special class of complex ceramic oxides called fluorites is able to resist this fate. The fundamental principle is rather simple: the configurations of atomic arrangements in these oxides are relatively disordered to begin with allowing them to tolerate displaced atoms caused by radiation.
- *Brilliant X-Rays Shine Light on Welds.* Using high-brightness synchrotron radiation, the details of microstructural changes of welds were mapped and studied for the first time. This advanced capability shows how the welding process alters the structure and changes the properties of metals. Its application is virtually unlimited, since it can investigate dynamic changes in crystal structure near the melting point of any metal. Knowledge gained from this award winning work on titanium and stainless steels is being used to advance and refine theories and numerical models of welding fundamentals. Dramatic savings to the U. S. economy would result from better quality, more reliable welds.
- *Micro Lens for Nano Research.* A silicon lens that is 1/10 the diameter of a human hair has been fabricated and used to image microscopic structures with an efficiency 1,000 times better than existing probes. The combination of high optical efficiency and improved spatial resolution over a broad range of wavelengths has enabled measurement of infrared light absorption in single biological cells. This spectroscopic technique can provide important information on cell chemical composition, structure, and biological activity.
- *Nanofluids.* Nanofluids (tiny, solid nanoparticles suspended in fluid) have been created that conduct heat ten times faster than thought possible, surpassing the fundamental limits of current heat conduction models for solid/liquid suspensions. These nanofluids are a new, innovative class of heat transfer fluids and represent a rapidly emerging field where nanoscale science and thermal engineering meet. This research could lead to a major breakthrough in making new composite (solid and liquid) materials with improved thermal properties for numerous engineering and medical

applications to achieve greater energy efficiency, smaller size and lighter weight, lower operating costs, and a cleaner environment.

### Chemical Sciences, Geosciences, and Energy Biosciences

- *Capturing Molecules in Motion with Synchrotron X-Ray Pulses.* Photochemical conversion of solar energy depends on light-driven chemical reactions. Absorption of light ultimately leads to atomic rearrangements necessary to produce photochemical products. The intermediate molecular configurations created by absorption of light are short-lived and their structures are largely unknown. In novel experiments at the Advanced Photon Source, molecular structures of laser-generated reaction intermediates in solutions, having lifetimes as short as 28 billionth of a second, have been obtained. Future experiments are planned that will allow for capture of intermediate structures on even shorter time scales. These studies are providing the fundamental knowledge needed to develop artificial photoconversion devices.
- *Early Precursor Identified in Water Radiolysis.* Radiolytic decomposition of water produces hydrogen gas, which is flammable and potentially explosive. This is of concern in maintenance of water-moderated nuclear reactors, long-term storage of transuranic fissile materials containing adsorbed water, and management of high-level mixed-waste storage tanks. In recent studies on the effects of ionizing radiation on condensed media, a common precursor to essentially all hydrogen from irradiated water has been discovered. This precursor is a solvated electron. External intervention and capture of this precursor can prevent the generation of hydrogen gas from water. The reactivity of the precursor with a large number of scavengers has previously been determined in pulse radiolysis experiments, thus a priori predictions can be made on the efficiency of the intervention and prevention of gas generation.
- *The World's Smallest Laser.* A team of materials scientists and chemists has built the world's smallest laser - a nanowire nanolaser 1,000 times thinner than a human hair. The device, one of the first to arise from the field of nanotechnology, can be tuned from blue to deep ultraviolet wavelengths. Zinc oxide wires only 20 to 150 nanometers in diameter and 10,000 nanometers long were grown, each wire a single nanolaser. Discovering how to excite the nanowires with an external energy source was critical to the success of the project. Ultimately, the goal is to integrate these nanolasers into electronic circuits for use in "lab-on-a-chip" devices that could contain small laser-analysis kits or as a solid-state, ultraviolet laser to allow an increase in the amount of data that can be stored on high-density optical disks.
- *Polymerization to Make Plastics.* The discovery of metallocene catalysts caused major advances in polymer production (e.g., polyethylene, polypropylene), the most widespread of synthetic materials. The ability to control the orientation of each link of a polymer chain allows control of crystallinity, density, softening point, and other important properties. A recent improvement in these catalysts is the synthesis of bimetallic complexes in which two catalytic centers and two cocatalytic centers are held in close proximity in solution or adsorbed on surfaces. By altering the nature of the centers, it is possible to control rate of reactivity, the degree of chain branching, and plastic rigidity.
- *First Ever Chemistry with Hassium, Element 108.* Element 108 - hassium - was discovered in 1984. It does not exist in nature but must be created one atom at a time by fusing lighter nuclei. Recently, the first experiments to examine its chemical properties were performed by an international team (German, Swiss, Russian, Chinese and American scientists) at the Gesellschaft für Schwerionenforschung (GSI) in Darmstadt, Germany using novel techniques developed at the Lawrence Berkeley National Laboratory. Energetic magnesium projectiles bombarded targets of

curium, a rare artificial isotope produced and processed at Oak Ridge National Laboratory. The hassium atoms formed by impacts between beam and target reacted with oxygen to form hassium oxide molecules enabling the study of the properties of this new chemical compound. The chemistry of man-made and heavy elements, particularly chemistry impacting environmental insults, is of major interest, and these experiments are a first step for this element.

- *Improved Materials for Fuel Cells.* Major impediments for the commercialization of fuel cells include the inability to use hydrogen fuel containing traces of carbon monoxide and the necessity of using large amounts of expensive platinum catalysts. A novel ruthenium/platinum catalyst has been produced through a new preparation method involving spontaneous deposition of platinum on metallic ruthenium nanoparticles. The resulting catalyst has a higher carbon monoxide tolerance than commercial catalysts and uses smaller amounts of platinum.
- *Platinum Encrusted Diamond Films.* Research on new catalytic electrodes, e.g., for fuel cells, has shown that synthetic diamond thin films are excellent supports for catalysts because of their corrosion resistance. The challenge to produce an electrode is to incorporate nanometer sized platinum and platinum/ruthenium catalyst particles into the surface structure of the diamond film. Recently, the ability to incorporate 10 to 500 nanometer diameter particles into the bulk structure of the films has been demonstrated. These new surface modified systems may result in significantly improved catalytic activity and stability, and could have even broader applications in chemical synthesis, toxic waste remediation, and chemical and biomedical sensors.
- *Complex Flow in the Subsurface.* Recovery of subsurface fluids, whether oil and gas or contaminants, requires understanding the way fluids flow within porous and fractured rocks and soil. This is particularly complicated when there are multiple fluids (oil-methane-water; water-carbon dioxide). New experiments combined with theory and computational modeling have tracked the simultaneous flow of two fluids in fractured and porous media. Flow paths of both fluids are significantly longer than under single fluid conditions and transport is very sensitive to differences in fluid structure.
- *Complete Plant Genome of the First Model Plant.* The first complete sequencing of a plant genome was completed by an international consortium of researchers from Europe, Japan and the U.S. The DOE was one of the supporters of the U.S. effort. The sequencing of the genome of Arabidopsis will provide the information needed to increase food production in an energy-efficient and environmentally friendly manner, provide increased wood and fiber production, and increase the use of plant materials for energy and the production of petroleum-replacing chemicals.



## Selected FY 2001 Facility Accomplishments

The four synchrotron radiation light sources and three BES neutron scattering facilities served 6,982 users in FY 2001 by delivering a total of 26,476 operating hours to 204 beam lines at an average of 96.1% reliability (delivered hours/scheduled hours)<sup>a</sup>. The High Flux Isotope Reactor at Oak Ridge National Laboratory did not operate in FY 2001 due to the installation of upgrades. Statistics for individual facilities are provided below. In one instance, less time was needed for maintenance activities than was scheduled, so more time was delivered to users than planned.

The maximum number of total operating hours for these 7 facilities is estimated to be about 37,100 hours. Most of the BES facilities already operate close to the maximum number of hours possible for their facility. The next priority is to support and maintain beamlines and instruments at the state-of-the-art. For the synchrotron radiation light sources and the neutron scattering facilities, the number of beamlines and instruments would need to be increased in order to achieve the full capacity of each of the facilities. Capacity at the light sources could increase by nearly a factor of two if all beamlines were fully instrumented. Capacity at the neutron sources could also increase substantially by upgrading existing instruments and fabricating new ones. These needs are addressed in the current request.

- **The Advanced Light Source (ALS)** served 1,163 users in FY 2001 by delivering 5,261 operating hours to 37 beam lines at 96.2% reliability (delivered hours/scheduled hours). The ALS is supported by the Materials Sciences and Engineering subprogram.
  - ▶ *A new beamline for x-ray microscopy of polymers.* Owing to its elemental and chemical specificity, x-ray microscopy is a superior tool for the study of multicomponent polymers. A scanning x-ray microscope that is specifically optimized to the demands of polymer research is being commissioned.
  - ▶ *Ambient-pressure photoemission spectroscopy.* The real world of chemistry, biology, and environmental science is a world that is frequently wet, hot, and under atmospheric or higher pressures, whereas experimental measurements are often best done under vacuum with cold samples. One step toward bridging the gap is the development of a new experimental chamber for *in-situ* investigation of samples under ambient conditions.
  - ▶ *Interferometer controls scanning x-ray microscope.* In scanning microscopy, it is essential to locate and control the position of the probe over the sample. A control system developed for a scanning x-ray microscope is able to position the x-ray beam with nanometer accuracy, so that features in the sample can be studied at the finest spatial resolution of the instrument.

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<sup>a</sup> BES defines "users" as researchers who conduct experiments at a facility (e.g., received a badge) or receive primary services from a facility. An individual is counted as one user per year regardless of how often he or she uses a given facility in a year. "Operating hours" are the total number of hours the facility delivers beam time to its users during the Fiscal Year. Facility operating hours are the total number of hours in the year (e.g., 365 days times 24 hour/day = 8,760 hours) minus time for machine research, operator training, accelerator physics, and shutdowns (due to maintenance, lack of budget, faults, safety issues, holidays, etc.).

- ▶ *Superbend beamlines developed.* To broaden the spectral range of the Advanced Light Source to cover shorter wavelengths, superconducting bend magnets were designed. The first two beamlines will be implemented sequentially over the next year to serve protein crystallographers and to provide much needed harder x-ray sources for ALS diffraction studies.
- **The Advanced Photon Source (APS)** served 1,989 users in FY 2001 by delivering 4,788 operating hours to 37 beam lines at 95.8% reliability (delivered hours/scheduled hours). The APS is supported by the Materials Sciences and Engineering subprogram.
  - ▶ *Storage ring “top-up operation” becomes routine.* After successful tests with 25% of the scheduled user-beam time dedicated to top-up operation, the APS is scheduling the majority of future operations for top-up mode. During top-up operation, injecting a pulse of electrons once every two minutes holds the stored current constant to 0.2 percent. This operating mode delivers a constant heat load on x-ray optics and various accelerator components, thus improving the x-ray beam stability. It also allows flexibility in operating modes, which are traditionally limited by the short lifetime of the stored beam. Top-up operation has significantly enhanced the research capabilities of the APS.
  - ▶ *Two undulators on a single straight section deliver two independent x-ray beams to users.* For the first time, a novel concept of spatially separating the beams from two insertion devices placed on single straight section was realized. This was accomplished by placing the undulator axes at a small angle with respect to each other. Successful implementation of this concept enabled 100% efficient utilization of the delivered beam.
  - ▶ *Low-emittance lattice developed.* Machine studies have successfully established operating conditions for the APS storage ring with the horizontal emittance reduced by approximately a factor of two. This reduces the horizontal source size and divergence of the x-ray beam and results in at least a factor of two improvement in the overall brilliance. Initial user results are encouraging and routine operation with this mode is scheduled for the near future.
- **The National Synchrotron Light Source (NSLS)** served 2,523 users in FY 2001 by delivering 5,556 operating hours to 86 beam lines at 100.0% reliability (delivered hours/scheduled hours). The NSLS is supported by the Materials Sciences and Engineering subprogram.
  - ▶ *Polarization modulation spectroscopy for magnetism research.* A new high-resolution soft x-ray beamline and a phase sensitive detection system were completed to take advantage of the fast switching capability of the Elliptically Polarized Wiggler. The new system provides high sensitivity and enables magnetic field dependent studies.
  - ▶ *Focusing of high energy x-rays with asymmetric Laue crystals.* Theoretical prediction and experimental verification of a new concept for focusing of high energy x-rays was demonstrated. This new design results in a more than 100 fold increase in the photon flux delivered to the sample. A new monochromator based on this design was constructed and implemented at the superconducting wiggler beamline for high pressure and materials research.
  - ▶ *High magnetic field, far-infrared spectroscopy beamline commissioned.* A new high magnetic field, far-infrared beamline was commissioned with a far-infrared spectrometer and 16 Tesla superconducting magnet. Combining this with a high-field magnet system opens up new

opportunities for measuring electron spin resonance (ESR), cyclotron resonance, and other magneto-optic effects in solids.

- ▶ *X-ray optics for microbeam diffraction, elemental mapping, and high pressure research developed.* A new system for micro-focusing of x-rays was implemented, achieving a focus of 3 microns (vertical) by 9 microns (horizontal). The system has been used in the study of bone diseases, materials under high pressure, and semiconductors.
- ▶ *High gain harmonic generation (HGFG) free electron laser (FEL) achieves saturation.* By frequency multiplying and amplifying a seed laser signal, an HGFG FEL imposes the properties of the laser onto the FEL output beam. In a demonstration, light at long wavelength was frequently doubled. Full characterization of the FEL light and its harmonics agreed with theory and demonstrated the utility of an HGFG FEL for producing intense coherent light pulses.
- **The Stanford Synchrotron Radiation Laboratory (SSRL)** served 907 users in FY 2001 by delivering 4,539 operating hours to 25 beam lines at 94.9% reliability (delivered hours/scheduled hours). The SSRL is supported by Materials Sciences and Engineering subprogram.
  - ▶ *Stanford-Berkeley synchrotron radiation summer school.* The first Stanford-Berkeley summer school on synchrotron radiation and its applications was held with 36 students from a diverse range of scientific fields. The goal was to introduce young scientists to the fundamental properties of synchrotron radiation and the understanding and use of several techniques, including spectroscopy, scattering, and microscopy.
  - ▶ *New actinide facility commissioned.* Synchrotron-based measurements are a crucial part of chemical and materials research programs involving radionuclides and radiologic materials. In order not to limit the scope of experiments that can be performed, a radiologic sample analysis facility has been integrated into a modern synchrotron beamline. This combination insures safe handling of actinide and other radiology materials and also provides state-of-the-art measurement capabilities that have proven extremely useful in remediation efforts.
  - ▶ *Materials science small angle x-ray scattering beamline facility completed.* The materials science small and wide-angle x-ray scattering station is now in full user operation. The integrated beamline and experimental equipment facility allows for studies of weakly scattering systems, such as dilute polymer solutions.
  - ▶ *Microfocus optics system for X-ray micro-spectroscopy.* An experimental apparatus employing tapered metal capillary optics for conducting X-ray micro-spectroscopy is now in operation. This capability allows X-ray micro-spectroscopy experiments in the materials, biological, and environmental sciences.
  - ▶ *Successful 3 GeV injector test.* The SPEAR injector was successfully run at 3 GeV, proving that it is ready to provide at-energy injection for SPEAR3. The 3 GeV test came toward the end of the two-year Injector Upgrade Accelerator Improvement Project, in which power supplies, magnets, and diagnostics were upgraded to insure reliable 3 GeV operation. At-energy injection will improve SPEAR3 performance by providing better fill-to-fill orbit reproducibility and thermal stability.

- ▶ *RF waveguide dampers improve beam stability and lifetime.* RF waveguide dampers were installed in the two radio frequency (RF) waveguides in the SPEAR storage ring to eliminate high frequency oscillations excited by the electron beam in the RF cavity/waveguide system. The dampers not only eliminated the instabilities but they allowed the use of operations parameters that gave a 20% improvement in the electron beam lifetime.
- **The Intense Pulsed Neutron Source (IPNS)** served 240 users in FY 2001 by delivering 3,968 operating hours to 13 beam lines at 102.6% reliability (delivered hours/scheduled hours). The IPNS is supported by the Materials Sciences and Engineering subprogram.
  - ▶ *IPNS hosts the national neutron and x-ray scattering school.* In August 2001, Argonne National Laboratory again hosted the two-week National School on Neutron and X-Ray Scattering. The school continues to attract outstanding graduate students and post-doctoral appointees with 179 applications for the 60 available positions.
  - ▶ *Upgrade of IPNS instruments.* The High Resolution Medium Energy Chopper Spectrometer (HRMECS) instrument was completely upgraded and a chopper was added to the General Purpose Powder Diffractometer (GPPD). The HRMECS upgrade included the complete overhaul of data collection/control software and hardware, addition of position-sensitive detectors at low scattering angles and improved neutron choppers. The T0 chopper on GPPD blocks high energy neutron from entering the diffractometer.
  - ▶ *Auto-anneal capabilities added to moderator system.* Regular annealing required for IPNS's unique ultra-cold moderator has been accomplished by installing a system that automatically anneals the solid methane moderator every three days. This automation allows for reduced manpower and improved operation of the IPNS target moderator assembly.
- **The Manuel Lujan Jr. Neutron Scattering Center at the Los Alamos Neutron Science Center** LANSCE served 122 users in FY 2001 by delivering 2,364 operating hours to 6 beam lines at 82.0% reliability (delivered hours/scheduled hours). The Lujan Center is supported by the Materials Sciences and Engineering subprogram.
  - ▶ *HIPPO diffractometer commissioned.* Following three years of design and construction, the recently completed HIPPO (High Pressure, Preferred Orientation) diffractometer took its first neutron-beam-related diffraction pattern on a sample of nickel on July 7, 2001. The scientific thrust of this new state-of-the-art spectrometer is the investigation of dynamic processes in heterogeneous bulk materials in a variety of environments.
  - ▶ *SMARTS will provide new capabilities in materials research.* SMARTS, a third generation neutron diffractometer for the study of polycrystalline materials, received its load frame and furnace, which were successfully tested onsite during 2001. SMARTS is scheduled to receive first beam in August 2001, followed by commissioning through the remainder of the year.
  - ▶ *BES partners on new institutional instruments.* Three institutionally funded instruments, ASTERIX, PHAROS, and IN500 were supported in part under the auspices of BES. ASTERIX produces a highly polarized intense beam of cold neutrons that has a very large cross section and covers a wide wavelength range while minimizing the fraction of the neutron beam that is not used. PHAROS, a high-resolution chopper spectrometer, is designed for low-angle studies.

IN500 is a cold neutron time-of-flight spectrometer, which will offer all the advantageous capabilities of reactor-based instruments.

- ▶ *Instrument performance improves with use of new chopper technology.* All of the Lujan Center's new instruments and some of the existing instruments have enjoyed dramatic improvements in chopper technology in FY 2001. These performance improvements in two technical areas, timing reference generators and chopper controls, now enable the accelerator and all neutron choppers to run as slaves of the master timing generator. This success in chopper technology has drawn the attention of several other spallation neutron facilities and has redefined the timing specifications for the Spallation Neutron Source.
  - ▶ *Upgrades to small-angle scattering instrument.* A new frame-overlap chopper was procured and installed, which enables the small-angle scattering instrument, LQD, to make full use of the higher flux it enjoys from the hydrogen moderator installed over the last two years. Recent additions to LQD also include a gravity-focusing device, which compensates for gravitational drop, especially for slow neutrons.
  - ▶ *Upgrades to SPEAR improve instrument performance.* SPEAR (Surface Profile Analysis Reflectometer) is used for determining chemical density profiles at solid/solid, solid/liquid, solid/gas, and liquid/gas interfaces. Upgrades to SPEAR during 2001 included the installation of shutter hardware to reduce closure time, and additional automation of flight-path components. For better performance, an evacuated flight path, and two digital chopper controllers were added. In addition, a new collimation system, together with improved software, allowed for the first real-time reflectivity measurements. These upgrades were made to make the instrument user-friendlier.
- **The High Flux Isotope Reactor (HFIR)** served 38 users in FY 2001 by delivering 8 operating hours for materials irradiation and institutes that utilize the transplutonium program and medical isotopes. The reactor was shut down at 8:00 a.m. on October 1, 2000, for the scheduled replacement of the beryllium reflector and installation of upgrades and remained shutdown for the remainder of the year. The HFIR is supported by the Materials Sciences and Engineering subprogram.
- ▶ *Installation of new components enhances scientific capabilities at HFIR.* Many of HFIR's internal components have been replaced with new, upgraded components that will significantly enhance its neutron scattering research capabilities without diminishing its isotope-production or material-testing capabilities. Replaced components include the beryllium reflector, its support structure, and three of the four neutron beam tubes. Beam intensity for some instruments is expected to be three times that of the original design.
  - ▶ *Cold Source Project progress.* The moderator vessel has been fabricated and has passed acceptance pressure tests at room and liquid-nitrogen temperatures.
  - ▶ *Spectrometers for cold neutron research.* The cold source to be installed at HFIR will provide long wavelength neutron beams that are unsurpassed worldwide. Instrumentation has been designed to make optimum use of the cold neutron beams. Instruments include small angle spectrometers for measurements on large-scale structures, reflectometers for the study of surface phenomena, and triple-axis spectrometers for the determination of low-energy excitations.

- ▶ *Spectrometers for thermal neutron research.* The larger beam tubes and new monochromator drums installed at HFIR will permit considerable gains in intensity for the thermal neutron spectrometers, by as much as a factor of five.
- **The Combustion Research Facility (CRF)** is supported by the Chemical Sciences, Geosciences, and Energy Biosciences subprogram.
  - ▶ *New capabilities.* The CRF provides a primary interface for the integration of BES programs with those of DOE's Offices of Energy Efficiency and Renewable Energy and Fossil Energy related to combustion by collocating basic and applied research at one facility. Three laboratories were completed. The particle diagnostic laboratory can now generate flames with controllable fuel and oxidizer feeds to develop a fundamental understanding of small particle formation from combustion sources. A time-resolved fourier transform spectrometer for chemical kinetics and dynamics studies is now available in the kinetics and mechanisms laboratory. Related to applied research, the investigation of a novel engine combustion concept is being conducted in the new homogeneous-charge, compression-ignition engine laboratory.

### Program Shifts

In FY 2003, the engineering activity of the formerly separate Engineering and Geosciences subprogram becomes part of the Materials Sciences and Engineering subprogram. The geosciences activity of the formerly separate Engineering and Geosciences subprogram and the Energy Biosciences subprogram become part of the Chemical Sciences, Geosciences, and Energy Biosciences subprogram. This directly aligns Basic Energy Sciences program management and organizational structures.

#### Materials Sciences and Engineering

- *Initiation of new activities in nanoscale science, engineering, and technology (NSET).* The FY 2001 NSET laboratory solicitation resulted in six awards including: Lawrence Berkeley National Laboratory in the areas of self assembly of organic/inorganic nanocomposite materials and the design, synthesis, characterization, and applications of functionalized nanotubes; Oak Ridge National Laboratory in the area of self-organized and artificially structured nanoscale materials, with emphasis on neutron scattering; Brookhaven National Laboratory in the area of electron microscopy applied to nanoscale structures; Los Alamos National Laboratory in the area of electronics from nanoscale crystals; and Sandia National Laboratories in the area of nanoelectronics and nanophotonics. The FY 2001 NSET university solicitation resulted in 35 grants.
- *Initiation of new activities in Robotics and Intelligent Machines (RIM).* The FY 2001 RIM university solicitation resulted in four grants for fundamental studies of automated sensing, perception, learning, and action.

#### Chemical Sciences, Geosciences, and Energy Biosciences

- *Initiation of new activities in nanoscale science, engineering, and technology (NSET).* The FY 2001 NSET laboratory solicitation resulted in six awards including: Argonne National Laboratory in the area of integrating the biomolecule - inorganic interface to build functional materials; Brookhaven National Laboratory in the areas of understanding the chemical reactivity of nanoparticle surfaces and research on electron and photon transfer through molecules connecting nanoparticles; National Renewable National Laboratory in the area of quantum dot communication through proteins and

nanotubes; Oak Ridge National Laboratory in the area of research on templated synthesis and reactivity of nanoparticles for energy and environmentally demanding reactions; and Lawrence Berkeley National Laboratory in the area of designing nanoparticle surfaces for controlling reaction selectivity. The FY 2001 NSET university solicitation resulted in 41 grants.

- *Initiation of new research in computational chemistry as part of the Scientific Discovery through Advanced Computing (SciDAC) activities.* The FY 2001 SciDAC laboratory solicitation resulted in awards to Ames Laboratory in the area of advancing multi-reference methods in electronic structure theory; Pacific Northwest National Laboratory and Lawrence Berkeley National Laboratory in the area of advanced methods for electronic structure; Sandia National Laboratory in the area of computation of reacting flows; and Argonne National Laboratory and Sandia National Laboratory for advanced software for the calculation of thermochemistry, kinetics and dynamics. The FY 2001 SciDAC university solicitation for computational chemistry resulted in 10 grants.

## **Scientific Facilities Utilization**

The BES program request includes \$313,887,000 to maintain support of the scientific user facilities. Research communities that have benefited from these facilities include materials sciences, condensed matter physics, chemical sciences, earth and geosciences, environmental sciences, structural biology, superconductor technology, medical research, and industrial technology development. The level of operations will be equal to that in FY 2002. More detailed descriptions of the specific facilities and their funding are given in the subprogram narratives and in the sections entitled Site Description and Major User Facilities.

## **Nanoscale Science Research**

In FY 2003, fundamental research to understand the properties of materials at the nanoscale will be increased in three areas: synthesis and processing of materials at the nanoscale; condensed matter physics; and catalysis. In the area of synthesis and processing (Materials Sciences and Engineering subprogram), new activities will develop a fundamental understanding of nanoscale processes involved in deformation and fracture, synthesis of ordered arrays of nanoparticles using patterning techniques, and synthesis of nanoparticles of uniform size and shape. In the area of condensed matter physics (Materials Sciences and Engineering subprogram), new activities will focus on understanding how properties change or can be improved at the nanoscale and how macromolecules reach their equilibrium configuration and self assemble into larger structures. In the area of catalysis (Chemical Sciences, Geosciences, and Energy Biosciences subprogram), new work will focus on fundamental research to understand the role nanoscale properties of materials play in altering and controlling catalytic transformations. In FY 2003, requests for applications in these research areas will be issued to DOE laboratories and to universities. The combination in a single coordinated research program of individual investigators at universities and interdisciplinary groups at the Department's laboratories is a proven excellent mechanism for incorporating advanced basic research, cutting-edge instrumentation, access to facilities, and the needs of energy technologies.

In addition to the increases for research in FY 2003, construction will begin on one Nanoscale Science Research Center (NSRC), and engineering and design will continue on two others. NSRCs are user facilities for the synthesis, processing, fabrication, and analysis of materials at the nanoscale. NSRCs were conceived in FY 1999 within the context of the NSTC Interagency Working Group on Nanoscale Science, Engineering, and Technology as part of the DOE contribution to the National Nanotechnology

Initiative. They involve conventional construction of a simple laboratory building, usually sited adjacent to or near an existing BES synchrotron or neutron scattering facility. Contained within NSRCs will be clean rooms; chemistry, physics, and biology laboratories for nanofabrication; and one-of-a-kind signature instruments and other instruments, e.g., nanowriters and various research-grade probe microscopies, not generally available outside of major user facilities. NSRCs will serve the Nation's researchers broadly and, as with the existing BES facilities, access to NSRCs will be through submission of proposals that will be reviewed by mechanisms established by the facilities themselves. Planning for the NSRCs includes substantial participation by the research community through a series of open, widely advertised workshops. Workshops held to date have been heavily attended, attracting up to 300 researchers. Funds are requested for the start of construction of the NSRC located at Oak Ridge National Laboratory and for the continuation of engineering and design for the NSRC located at Lawrence Berkeley National Laboratory and the NSRC at Sandia National Laboratories (Albuquerque) and Los Alamos National Laboratory. These NSRCs were chosen from among those proposed by a peer review process. Additional information on the NSRCs is provided in the construction project data sheet, project number 03-R-312 and in the PED data sheet, project number 02-SC-002.

The research efforts described in the first paragraph above will benefit significantly from these NSRCs. For example, the NSRC at Oak Ridge National Laboratory will provide direct access to sample preparation for neutron scattering, which is ideal for magnetic structures and for soft materials and residual stress in materials; Oak Ridge also has a combination of electron beam microcharacterization instruments that are needed to characterize nanoscale particles and dislocations. The NSRC at Lawrence Berkeley National Laboratory will provide synthesis capabilities to explore the phenomena of macromolecular conformation and assembly and will provide ready access to the Advanced Light Source and other characterization instruments. The NSRC at Sandia/Los Alamos National Laboratories will provide sample preparation capabilities for thin films, electron transport, patterning, and magnetic layered structures. This NSRC will also have an array of characterization instruments for nanoelectronics, thin films, and magnetic structures; in the case of magnetic materials, the NSRC will provide ready access to the National High Magnetic Field Laboratory at Los Alamos.

This research activity will also benefit by new work proposed in FY 2003 in the Advanced Scientific Computing Research (ASCR) program in the area of computational nanoscale science engineering and technology. ASCR will develop the specialized computational tools for nanoscale science.

## **Spallation Neutron Source (SNS) Project**

The purpose of the SNS Project is to provide a next-generation short-pulse spallation neutron source for neutron scattering. The SNS will be used by researchers from academia, national and federal labs, and industry for basic and applied research and for technology development in the fields of condensed matter physics, materials sciences, magnetic materials, polymers and complex fluids, chemistry, biology, earth sciences, and engineering. When completed in 2006, the SNS will be significantly more powerful (by about a factor of 10) than the best spallation neutron source now in existence -- ISIS at the Rutherford Laboratory in England. The facility will be used by 1,000-2,000 scientists and engineers annually. Interest in the scientific community in the SNS is increasing.

In FY 2001, two grants were awarded to universities for research requiring the design, fabrication, and installation of instruments for neutron scattering. These instruments will be sited at the SNS, with commissioning beginning late in FY 2006, shortly after the SNS facility itself is commissioned. Both awards were made based on competitive peer review conducted under 10 CFR Part 605, Financial



Assistance Program. An interagency working group was established under the auspices of the Office of Science and Technology Policy to coordinate the funding neutron scattering instruments at all of the neutron sources in view of the opportunity for new instruments at SNS. In addition to these two instruments, the BES program will provide \$5,000,000 of Materials Sciences and Engineering subprogram funding for continuing the development of instruments to exploit the scientific potential of the SNS facility. These instruments will be built by individual DOE laboratories or consortia of DOE laboratories in collaboration with the SNS based on scientific merit and importance to users from universities, industries, and government laboratories.

Neutron scattering will play a role in all forms of materials research and design, including the development of smaller and faster electronic devices; lightweight alloys, plastics, and polymers for transportation and other applications; magnetic materials for more efficient motors and for improved magnetic storage capacity; and new drugs for medical care. The high neutron flux (i.e., high neutron intensity) from the SNS will enable broad classes of experiments that cannot be done with today's low-flux sources. For example, high flux enables studies of small samples, complex molecules and structures, time-dependent phenomena, and very weak interactions.

The SNS will consist of a linac-ring accelerator system that delivers short (microsecond) proton pulses to a target/moderator system where neutrons are produced by a process called spallation. The neutrons so produced are then used for neutron scattering experiments. Specially designed scientific instruments use these pulsed neutron beams for a wide variety of investigations. There will initially be one partially instrumented target station with the potential for adding more instruments and a second target station later.

The SNS project partnership among six DOE laboratories takes advantage of specialized technical capabilities within the laboratories: Lawrence Berkeley National Laboratory in ion sources; Los Alamos National Laboratory in linear accelerators; Thomas Jefferson National Accelerator Facility in superconducting linear accelerators; Brookhaven National Laboratory in proton storage rings; Argonne National Laboratory in instruments; and Oak Ridge National Laboratory in targets and moderators.

The SNS project has made progress during FY 2001 and the project continues to meet scheduled milestones and remains within budget. Project-wide, design work is about two-thirds complete, and R&D on technical components is nearing completion. Title II design of conventional facilities is nearly 100% complete. Site preparation has cleared the way for construction of the front end and target buildings, the linac tunnel, and a number of support buildings and utility systems. Procurements for technical components have been awarded with generally favorable cost results, and deliveries of some items to Oak Ridge have begun. Definitive plans have been developed for equipment installation and facility commissioning activities.

FY 2002 budget authority has been provided to continue R&D, design, procurement, and construction activities, and to begin component installation. Essentially all R&D supporting the construction of the SNS will be completed in FY 2002, with instrument R&D continuing throughout the project. Title II design will be completed on the linac, and will continue on the ring, target, and instrument systems. Equipment installation efforts will begin in the front end and the low energy sections of the linac. Other technical components for the linac, ring, target, and instruments will continue to be manufactured. Work on conventional facilities will continue. Some conventional facilities will reach completion and be made available for equipment installation, such as the front end building, and portions of the klystron building and linac tunnel. Construction work will begin on the ring tunnel.

FY 2003 funding is requested to continue instrument R&D and design, procurement, construction, and installation activities, and to begin system commissioning. The front end will be commissioned, and low-energy linac component installation and commissioning will commence. Other linac and ring components will begin to be delivered and installed in their respective tunnels. Target building construction and equipment installation will continue in concert with each other. Numerous conventional facilities including the klystron, central utilities, and ring service buildings as well as the linac and ring tunnels will be completed. All site utilities will be available to support linac commissioning activities.

The estimated Total Project Cost remains constant at \$1,411,700,000 and the construction schedule continues to call for project completion by mid-2006. The estimate for annual operating costs has been updated to reflect more recent experience in the operation of major user facilities as well as in design, development, fabrication, maintenance, and user support of modern instruments. Additional information on the SNS Project is provided in the SNS construction project data sheet, project number 99-E-334.

### **The Linac Coherent Light Source (LCLS) Project**

The purpose of the Linac Coherent Light Source (LCLS) Project is to provide laser-like radiation in the x-ray region of the spectrum that is 10 orders of magnitude (i.e., a factor of 10,000,000,000) greater in peak power and peak brightness than any existing coherent x-ray light source. This advance in brightness is similar to that of a synchrotron over a 1960's laboratory x-ray tube. Synchrotrons have revolutionized science across disciplines ranging from atomic physics to structural biology. Advances from the LCLS are expected to be equally dramatic. The LCLS Project will provide the world's first demonstration of an x-ray free-electron-laser (FEL) in the 1.5 - 15 Å range.

For many years, the Basic Energy Sciences Advisory Committee (BESAC) has been actively involved with the development of such a next-generation light source. In 1997, the BESAC report *DOE Synchrotron Radiation Sources and Science* recommended funding an R&D program in next-generation light sources. In 1999, the BESAC report *Novel, Coherent Light Sources* concluded "Given currently available knowledge and limited funding resources, the hard x-ray region (8-20 keV or higher) is identified as the most exciting potential area for innovative science. DOE should pursue the development of coherent light source technology in the hard x-ray region as a priority. This technology will most likely take the form of a linac-based free electron laser using self-amplified stimulated emission or some form of seeded stimulated emission..."

The proposed LCLS will have properties vastly exceeding those of current x-ray sources in three key areas: peak brightness, coherence, and ultrashort pulses. The peak brightness of the LCLS is 10 orders of magnitude greater than current synchrotrons; the light is coherent or "laser like" enabling many new types of experiments; and the pulses are short (230 femtoseconds with planned improvements that will further reduce the pulse length) enabling studies of fast chemical and physical processes. These characteristics open new realms of scientific applications in the chemical, material, and biological sciences including fundamental studies of the interaction of intense x-ray pulses with simple atomic systems, structural studies on single nanoscale particles and biomolecules, ultrafast dynamics in chemistry and solid-state physics, studies of nanoscale structure and dynamics in condensed matter, and use of the LCLS to create plasmas.

The LCLS project leverages capital investments in the existing SLAC linac as well as technologies developed for linear colliders and for the production of intense electron beams with radio-frequency photocathode guns. The SLAC linac will provide high-current, low-emittance 5–15 GeV electron bunches at a 120 Hz repetition rate. When traveling through a newly constructed long undulator, the electron bunches will lead to self-amplification of the emitted x-ray radiation, constituting the x-ray FEL. The availability of the SLAC linac for the LCLS Project creates a unique opportunity (worldwide) for demonstration and use of x-ray FEL radiation.

The proposed LCLS Project requires a 150 MeV injector to be built at Sector 20 of the 30-sector SLAC linac to create the electron beam required for the x-ray FEL. The last one third of the linac will be modified by adding two magnetic bunch compressors. Most of the linac and its infrastructure will remain unchanged. The existing components in the Final Focus Test Beam tunnel will be removed and replaced by a new 120 meter undulator and associated equipment. The preliminary Total Estimated Cost (TEC) is in the range of \$165,000,000 to \$225,000,000. FY 2003 Project Engineering and Design (PED) funding of \$6,000,000 is requested for Title I and Title II design work. Additional information on the LCLS Project is provided in the LCLS PED data sheet, project number 03-SC-002.

### **Research Using X-ray and Neutron Scattering**

X-ray and neutron scattering are powerful tools used to investigate the fundamental properties of materials. BES is the major supporter of x-ray and neutron science in the United States and has pioneered the development of virtually all of the instruments and techniques used at these facilities for research in materials sciences, surface science, condensed matter physics, atomic and molecular physics, chemical dynamics, x-ray microscopy, tomography, femtosecond phenomena, interfacial/environmental, and geophysics studies. Within the physical sciences, BES remains the dominant federal supporter of beamline development and instrument fabrication providing as much as 85% of the federal support for these activities.

Major instruments at the synchrotron light sources and the neutron sources have a lifetime of 7-10 years after which the instruments undergo major upgrades or are retired. Thus, after a facility is fully instrumented, about 10-15% of the instruments must be upgraded or replaced each year to keep the facility at the forefront of science. In FY 2003, new funding in the amount of \$17,292,000 is requested to support instrument upgrades, instrument replacements, and new instrumentation at the x-ray and neutron scattering facilities. Of these funds, \$5,000,000 will be provided for instruments at the Spallation Neutron Source. These funds will be competed among both academic and laboratory institutions, and the resulting instruments and beamlines will be made available to the entire U.S. scientific research community.

## **Workforce Development**

The BES program supports development of the R&D workforce through support of undergraduate researchers, graduate students working toward a doctoral degree, and postdoctoral associates developing their research and management skills. In addition, the BES scientific user facilities provide outstanding hands-on research experience to many young scientists. Thousands of students and post-doctoral investigators are among the 8,000 researchers who conduct experiments at BES-supported facilities each year. The work that these young investigators perform at BES facilities is supported by a wide variety of sponsors including BES, other Departmental research programs, other federal agencies, and private institutions. The R&D workforce developed under this program provides new scientific talent in areas of fundamental research and also provides talent for a wide variety of technical and industrial areas that require the problem solving abilities, computing skills, and technical skills developed through an education and experience in fundamental research.

This program supported graduate students and postdoctoral investigators in FY 2001 through grants or contracts; 4,046 graduate students and postdoctoral investigators used the BES science user facilities in FY 2001.

## Funding Profile

(dollars in thousands)

	FY 2001 Comparable Appropriation	FY 2002 Original Appropriation	FY 2002 Adjustments	FY 2002 Comparable Current Appropriation	FY 2003 Request
Basic Energy Sciences					
Research					
Materials Sciences and Engineering.....	511,608	434,353	+78,169	512,522	547,883
Chemical Sciences, Geosciences, and Energy Biosciences.....	203,231	218,714	-10,931	207,783	220,146
Engineering and Geosciences..	0	38,938	-38,938	0	0
Energy Biosciences .....	0	32,400	-32,400	0	0
Subtotal, Research.....	714,839	724,405	-4,100	720,305	768,029
Construction.....	258,929	279,300	0	279,300	251,571
Total, Basic Energy Sciences.....	973,768	1,003,705	-4,100	0	0
General Reduction .....	0	-4,100	4,100	0	0
Total, Basic Energy Sciences.....	973,768 <sup>a b</sup>	999,605	0	999,605	1,019,600

**Public Law Authorization:**

Public Law 95-91, "Department of Energy Organization Act"

Public Law 103-62, "Government Performance and Results Act of 1993"

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<sup>a</sup> Excludes \$15,962,000 which was transferred to the SBIR program and \$958,000 which was transferred to the STTR program.

<sup>b</sup> Excludes \$991,000 which was transferred to the Science Safeguards and Security program in an FY 2001 reprogramming.

## Funding by Site

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
<b>Albuquerque Operations Office</b>					
Los Alamos National Laboratory.....	24,205	22,738	23,041	+303	+1.3%
National Renewable Energy Laboratory...	5,876	5,247	4,562	-685	-13.1%
Sandia National Laboratory .....	24,673	23,349	25,987	+2,638	+11.3%
<b>Total, Albuquerque Operations Office .....</b>	<b>54,754</b>	<b>51,334</b>	<b>53,590</b>	<b>+2,256</b>	<b>+4.4%</b>
<b>Chicago Operations Office</b>					
Ames Laboratory .....	17,961	16,114	16,507	+393	+2.4%
Argonne National Laboratory – East .....	159,028	154,389	152,734	-1,655	-1.1%
Brookhaven National Laboratory .....	75,942	56,606	57,398	+792	+1.4%
Chicago Operations Office.....	110,664	88,266	84,204	-4,062	-4.6%
<b>Total, Chicago Operations Office .....</b>	<b>363,595</b>	<b>315,375</b>	<b>310,843</b>	<b>-4,532</b>	<b>-1.4%</b>
<b>Idaho Operations Office</b>					
Idaho National Engineering and Environmental Laboratory.....	2,660	1,756	1,494	-262	-14.9%
<b>Oakland Operations Office</b>					
Lawrence Berkeley National Laboratory...	77,896	74,649	78,691	+4,042	+5.4%
Lawrence Livermore National Laboratory..	5,643	4,793	4,676	-117	-2.4%
Stanford Linear Accelerator Center (SSRL).	34,691	31,643	41,716	+10,073	+31.8%
Oakland Operations Office .....	43,433	36,973	34,497	-2,476	-6.7%
<b>Total, Oakland Operations Office .....</b>	<b>161,663</b>	<b>148,058</b>	<b>159,580</b>	<b>+11,522</b>	<b>+7.8%</b>
<b>Oak Ridge Operations Office</b>					
Oak Ridge Institute For Science and Education.....	1,245	440	872	+432	+98.2%
Oak Ridge National Laboratory .....	374,386	391,333	343,176	-48,157	-12.3%
Oak Ridge Operations Office.....	39	0	0	0	--
<b>Total, Oak Ridge Operations Office .....</b>	<b>375,670</b>	<b>391,773</b>	<b>344,048</b>	<b>-47,725</b>	<b>-12.2%</b>
<b>Richland Operations Office</b>					
Pacific Northwest National Laboratory .....	13,024	11,346	11,648	+302	+2.7%
Washington Headquarters .....	2,402	79,963	138,397	+58,434	+73.1%
<b>Total, Basic Energy Sciences.....</b>	<b>973,768<sup>a b</sup></b>	<b>999,605</b>	<b>1,019,600</b>	<b>+19,995</b>	<b>+2.0%</b>

<sup>a</sup> Excludes \$15,962,000 which was transferred to the SBIR program and \$958,000 which was transferred to the STTR program.

<sup>b</sup> Excludes \$991,000 which was transferred to the Science Safeguards and Security program in an FY 2001 reprogramming.

## Site Description

### Ames Laboratory

Ames Laboratory is a Multiprogram Laboratory located on 10 acres in Ames, Iowa. The laboratory was built on the campus of Iowa State University during World War II to emphasize the purification and science of rare earth materials. This emphasis continues today. The BES Materials Sciences and Engineering subprogram supports experimental and theoretical research on rare earth elements in novel mechanical, magnetic, and superconducting materials. Ames scientists are experts on magnets, superconductors, and quasicrystals that incorporate rare earth elements. The BES Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports theoretical studies for the prediction of molecular energetics and chemical reaction rates. Ames Laboratory provides leadership in analytical and separations chemistry.

Ames Laboratory is home to the **Materials Preparation Center (MPC)**, which is dedicated to the preparation, purification, and characterization of rare-earth, alkaline-earth, and refractory metal and oxide materials. Established in 1981, the MPC is a one-of-a-kind resource that provides scientists at university, industrial, and government laboratories with research and developmental quantities of high-purity materials and unique analytical and characterization services that are not available from commercial suppliers. The MPC is renowned for its technical expertise in alloy design and for creating materials that exhibit ultrafine microstructures, high strength, magnets, and high conductivity. The MPC also operates the Materials Referral System and Hotline, where users may obtain free information from a database of over 2,500 expert sources for the preparation and characterization of a wide variety of commercial materials and research samples.

### Argonne National Laboratory

Argonne National Laboratory (ANL) in Argonne, Illinois, is a Multiprogram Laboratory located on 1,700 acres in suburban Chicago. ANL has a satellite site located in Idaho Falls, Idaho. ANL is home to research activities in broad areas of materials and chemical sciences. It is also the site of three BES supported user facilities -- the Advanced Photon Source (APS), the Intense Pulsed Neutron Source (IPNS), and the Electron Microscopy Center for Materials Research (EMC).

The Materials Sciences and Engineering subprogram supports research in high-temperature superconductivity; polymeric superconductors; thin-film magnetism; surface science; the synthesis, advanced electron beam microcharacterization, and atomistic computer simulation of interfaces in advanced ceramic thin-films; defects and disordered materials; and synthesis and electronic and structural characterization of oxide ceramic materials, including high-temperature superconductors. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports research in actinide separations; physical and chemical properties of actinide compounds; structural aspects fundamental to advanced electrochemical energy storage; the chemistry of complex hydrocarbons; experimental and theoretical studies of metal clusters of catalytically active transition metals; molecular dynamics of gas-phase chemical reactions of small molecules and radicals; photosynthesis mechanisms; atomic, molecular, and optical physics; organic geochemistry related to hydrocarbon formation, and computational microtomography of porous earth materials. ANL has one of three pulsed radiolysis

activities that together form a national research program in this area. The other two are at Brookhaven National Laboratory and the University of Notre Dame.

The **Advanced Photon Source** is one of only three third-generation, hard x-ray synchrotron radiation light sources in the world, and it is the only one in the Americas. It is a world-class facility. Dedicated in 1996, the construction project was completed five months ahead of schedule and for less than the budget. The 7 GeV hard x-ray light source has since met or exceeded all technical specifications. For example, the APS is 10 times more brilliant than its original specifications and the vertical stability of the particle beam is three times better than its design goal. The 1,104-meter circumference facility -- large enough to house a baseball park in its center -- includes 34 bending magnets and 34 insertion devices, which generate a capacity of 68 independently controlled beamlines for experimental research. Beamlines are assigned to user groups in Collaborative Access Teams (CATs), whose proposals are reviewed and approved based on their scientific program and the criticality of high-brilliance x-rays to the work. These instruments attract researchers to study the structure and properties of materials in a variety of disciplines, including condensed matter physics, materials sciences, chemistry, geosciences, structural biology, medical imaging, and environmental sciences. The high-quality, reliable x-ray beams at the APS have already brought about new discoveries in materials structure.

The **Intense Pulsed Neutron Source** is a 30 Hz short-pulsed spallation neutron source that first operated all instruments in the user mode in 1981. Twelve neutron beam lines serve 14 instruments, one of which is a test station for instrument development. Distinguishing characteristics of IPNS include its innovative instrumentation and source technology and its dedication to serving the users. The first generation of virtually every pulsed source neutron scattering instrument was developed at IPNS. In addition, the source and moderator technologies developed at IPNS, including uranium targets, liquid hydrogen and methane moderators, solid methane moderators, and decoupled reflectors, have impacted spallation sources worldwide. A recent BESAC review of this facility described it as a “reservoir of expertise with a track record of seminal developments in source and pulsed source instruments second to none” and noted that ANL is “fully committed from top to bottom to supporting the user program.” This is reflected by a large group of loyal, devoted users. Research at IPNS is conducted on the structure of high-temperature superconductors, alloys, composites, polymers, catalysts, liquids and non-crystalline materials, materials for advanced energy technologies, and biological materials. The staff of the IPNS is taking a leadership role in the design and construction of instrumentation for the Spallation Neutron Source at Oak Ridge National Laboratory.

The **Electron Microscopy Center for Materials Research** provides in-situ, high-voltage and intermediate voltage, high-spatial resolution electron microscope capabilities for direct observation of ion-solid interactions during irradiation of samples with high-energy ion beams. The EMC employs both a tandem accelerator and an ion implanter in conjunction with a transmission electron microscope for simultaneous ion irradiation and electron beam microcharacterization. It is the only instrumentation of its type in the Western Hemisphere. The unique combination of two ion accelerators and an electron microscope permits direct, real-time, in-situ observation of the effects of ion bombardment of materials and consequently attracts users from around the world.



## **Brookhaven National Laboratory**

Brookhaven National Laboratory (BNL) is a Multiprogram Laboratory located on 5,200 acres in Upton, New York. BNL is home to BES major research efforts in materials and chemical sciences as well as to efforts in geosciences and biosciences. BNL is also the site of the National Synchrotron Light Source (NSLS).

The Materials Sciences and Engineering subprogram emphasizes experiments that make use of the NSLS. BNL scientists are among the world leaders in neutron and x-ray scattering applied to a wide variety of research problems such as high-temperature superconductivity, magnetism, structural and phase transformations in solids, and polymeric conductors. BNL has strong research programs in nanoscale structure and defects, the structure and composition of grain boundaries and interfaces, high temperature superconductors, and aqueous and galvanic corrosion.

The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports one of three national activities for pulsed radiolysis research at BNL. The innovative short-pulse radiation chemistry facility contributes to radiation sciences research across broad areas of chemistry. There is also research on the spectroscopy of reactive combustion intermediates and studies of the mechanisms of electron transfer related to artificial photosynthesis. Other chemistry research at BNL is focused around the unique capabilities of the NSLS in obtaining time dependant structural data of reacting systems, the structural changes accompanying catalytic and electrochemical reactions, the formation of atmospheric aerosols and their reactivity, and the interactions of rock-fluid systems. Biosciences research activities include mechanistic and molecular-based studies on photosynthesis, lipid metabolism, and genetic systems.

The **National Synchrotron Light Source** (NSLS) is among the largest and most diverse scientific user facilities in the world. The NSLS, commissioned in 1982, has consistently operated at >95% reliability 24 hours a day, seven days a week, with scheduled periods for maintenance and machine studies. Adding to its breadth is the fact that the NSLS consists of two distinct electron storage rings. The x-ray storage ring is 170 meters in circumference and can accommodate 60 beamlines or experimental stations, and the VUV storage ring can provide 25 additional beamlines around its circumference of 51 meters. Synchrotron light from the x-ray ring is used to determine the atomic structure of materials using diffraction, absorption, and imaging techniques. Experiments at the VUV ring help solve the atomic and electronic structure as well as the magnetic properties of a wide array of materials. These data are fundamentally important to virtually all of the physical and life sciences as well as providing immensely useful information for practical applications. The petroleum industry, for example, uses the NSLS to develop new catalysts for refining crude oil and making by-products like plastics.

The **High Flux Beam Reactor**, commissioned in 1965, was a research reactor designed to produce neutrons for scattering. During its three decades of operation, the HFBR was a premier gathering spot for neutron scientists involved in a broad array of studies, including phonons in rare gases; ferromagnets and antiferromagnets; critical phenomena in magnetic transitions; structure and dynamics of molecules adsorbed on surfaces; direct measure of electron-phonon interaction in 'old' superconductors; structure determination of small sub-unit of ribosomes; critical phenomena in one- and two-dimensional magnets; impurity effects on phase transitions; incommensurate systems in metals and insulators; magnetic correlations in heavy fermions; magnetic superconductors; hydrogen location in amino acids and carbohydrate building blocks; static and dynamic correlations in high temperature superconductors; exotic behavior of one-dimensional magnets; shape memory materials; anomalous correlation lengths in phase transitions; and the structure of ceramics with negative thermal expansion. In December 1996, a plume of tritiated water was discovered emanating from a leak in the HFBR spent fuel pool, which

contaminated the groundwater south of the reactor. The facility remained on standby until the Secretary of Energy announced on November 16, 1999, that the reactor would be permanently closed. Activities to place the reactor in a safe state awaiting full decommissioning by DOE's Office of Environmental Management were completed in FY 2001. The permanent shut down of the HFBR increases the importance of the remaining neutron sources in the U.S.

## **Idaho National Engineering and Environmental Laboratory**

Idaho National Environmental and Engineering Laboratory (INEEL) is a Multiprogram Laboratory located on 572,000 acres in Idaho Falls, Idaho. The Materials Sciences and Engineering subprogram supports studies to establish controls of biologically based engineering systems, to understand and improve the life expectancy of material systems used in engineering such as welded systems, and to develop new diagnostic techniques for engineering systems. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram focuses on fundamental understanding of negative ion mass spectrometry, studies of secondary ion mass spectrometry, and computer simulation of ion motion and configuration of electromagnetic fields crucial to the design of ion optics.

## **Lawrence Berkeley National Laboratory**

Lawrence Berkeley National Laboratory (LBNL) is a Multiprogram Laboratory located in Berkeley, California, on a 200-acre site adjacent to the Berkeley campus of the University of California. LBNL is home to BES major research efforts in materials and chemical sciences as well as to efforts in geosciences, engineering, and biosciences. Collocated with the University of California at Berkeley, the Laboratory benefits from regular collaborations and joint appointments with numerous outstanding faculty members. The Laboratory is the home to the research of many students and postdoctoral appointees. LBNL is also the site of two BES supported user facilities -- the Advanced Light Source (ALS) and the National Center for Electron Microscopy (NCEM).

The Materials Sciences and Engineering subprogram supports research in laser spectroscopy, superconductivity, thin films, femtosecond processes, x-ray optics, biopolymers, polymers and composites, surface science, theory, and nonlinear dynamics. Research is carried out on new aluminum-based alloys containing germanium and silicon; the structures of magnetic, optical, and electrical thin films and coatings; processing, mechanical fatigue, and high-temperature corrosion of structural ceramics and ceramic coatings; mechanical behavior of metals; and the synthesis, structure, and properties of advanced semiconductor and semiconductor-metal systems. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports fundamental, chemical dynamics research using molecular-beam techniques. Femtosecond spectroscopy studies of energy transfer on surfaces has also been developed. LBNL is recognized for its work in radiochemistry, the chemistry of the actinides, inorganic chemistry, and both homogeneous and heterogeneous chemical catalysis. Experimental and computational geosciences research is supported on coupled reactive fluid flow and transport properties and processes in the subsurface, and how to track and image them. In particular, geochemical studies focus on experimental and modeling studies on critical shallow earth mineral systems, improving analytical precision in synchrotron x-ray studies, and improving our understanding of how isotopic distributions act as tracers for geologic processes and their rates. Biosciences research focuses on the physics of the photosynthetic apparatus and on the formation of subcellular organelles.

The **Advanced Light Source** (ALS) began operations in October 1993 and now serves over 1,000 users as one of the world's brightest sources of high-quality, reliable vacuum-ultraviolet (VUV) light and long-wavelength (soft) x-rays. Soft x-rays and VUV light are used by the researchers at the ALS as high-resolution tools for probing the electronic and magnetic structure of atoms, molecules, and solids, such as those for high-temperature superconductors. The high brightness and coherence of the ALS light are particularly suited for soft x-ray imaging of biological structures, environmental samples, polymers, magnetic nanostructures, and other inhomogeneous materials. Other uses of the ALS include holography, interferometry and the study of molecules adsorbed on solid surfaces. The pulsed nature of the ALS light offers special opportunities for time resolved research, such as the dynamics of chemical reactions. Shorter wavelength (intermediate-energy) x-rays are also used at structural biology experimental stations for x-ray crystallography and x-ray spectroscopy of proteins and other important biological macromolecules. The ALS is a growing facility with a lengthening portfolio of beamlines that have already been applied to make important discoveries in a wide variety of scientific disciplines.

The **National Center for Electron Microscopy** provides instrumentation for high-resolution, electron-optical microcharacterization of atomic structure and composition of metals, ceramics, semiconductors, superconductors, and magnetic materials. This facility contains one of the highest resolution electron microscopes in the U.S.

The **Molecular Foundry**, a planned BES Nanoscale Science Research Center and a current PED project, will support research and the operation of a user facility for the design, modeling, synthesis, processing, fabrication and characterization of novel molecules and nanoscale materials. The facility will provide laboratories for materials science, physics, chemistry, biology, and molecular biology. State-of-the-art equipment will include a class 100 clean room, controlled environmental rooms, scanning tunneling microscopes, atomic force microscopes, transmission electron microscope, fluorescence microscopes, mass spectrometers, DNA synthesizer and sequencer, nuclear magnetic resonance spectrometer, ultrahigh vacuum scanning-probe microscopes, photo, uv, and e-beam lithography equipment, peptide synthesizer, advanced preparative and analytical chromatographic equipment, and cell culture facilities.

## **Lawrence Livermore National Laboratory**

Lawrence Livermore National Laboratory (LLNL) is a Multiprogram Laboratory located on 821 acres in Livermore, California. This laboratory was built in Livermore as a weapons laboratory 42 miles from the campus of the University of California at Berkeley to take advantage of the expertise of the university in the physical sciences. The Materials Sciences and Engineering subprogram supports research in positron materials science, superplasticity in alloys, adhesion and bonding at interfaces, kinetics of phase transformations in welds. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports plasma assisted catalysis for environmental control of pollutants, geosciences research on the source(s) of electromagnetic responses in crustal rocks, seismology theory and modeling, the mechanisms and kinetics of low-temperature geochemical processes and the relationships among reactive fluid flow, geochemical transport and fracture permeability.

## **Los Alamos National Laboratory**

Los Alamos National Laboratory (LANL) is a Multiprogram Laboratory located on 27,000 acres in Los Alamos, New Mexico. LANL is home to BES major research efforts in materials sciences with other efforts in chemical sciences, geosciences, and engineering. LANL is also the site of the Manuel Lujan Jr., Neutron Scattering Center at the Los Alamos Neutron Science Center (LANSCE).

The Materials Sciences and Engineering subprogram supports research on strongly correlated electronic materials, high-magnetic fields, microstructures, deformation, alloys, bulk ferromagnetic glasses, mechanical properties, ion enhanced synthesis of materials, metastable phases and microstructures, and mixtures of particles in liquids. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports research to understand the electronic structure and reactivity of actinides through the study of organometallic compounds. Also supported is work to understand the chemistry of plutonium and other light actinides in both near-neutral pH conditions and under strongly alkaline conditions relevant to radioactive wastes and research in physical electrochemistry fundamental to energy storage systems. In the areas of geosciences, experimental and theoretical research is supported on rock physics, seismic imaging, the physics of the earth's magnetic field, fundamental geochemical studies of isotopic equilibrium/disequilibrium, and mineral-fluid-microbial interactions.

The **Los Alamos Neutron Science Center** provides an intense pulsed source of neutrons for both national security research and civilian research. LANSCE is comprised of a high-power 800-MeV proton linear accelerator, a proton storage ring, production targets to the Manuel Lujan Jr. Neutron Scattering Center and the Weapons Neutron Research facility, and a variety of associated experiment areas and spectrometers. The Lujan Center features instruments for measurement of high-pressure and high-temperature samples, strain measurement, liquid studies, and texture measurement. The facility has a long history and extensive experience in handling actinide samples. A new 30 Tesla magnet is available for use with neutron scattering to study samples in high-magnetic fields.

The **Center for Integrated Nanotechnologies (CINT)**, a planned BES Nanoscale Science Research Center, will focus on exploring the path from scientific discovery to the integration of nanostructures into the micro- and macroworlds. This path involves experimental and theoretical exploration of behavior, understanding new performance regimes and concepts, testing designs, and integrating nanoscale materials and structures. CINT focus areas are nanophotonics and nanoelectronics, complex functional nanomaterials, nanomechanics, and the nanoscale/bio/microscale interfaces. CINT will be jointly administered by Los Alamos National Laboratory and Sandia National Laboratory. This Center will make use of a wide range of specialized facilities including the Los Alamos Neutron Science Center and the National High Magnetic Field Laboratory at LANL.

## **National Renewable Energy Laboratory**

National Renewable Energy Laboratory (NREL) is a program-dedicated laboratory (Solar) located on 300 acres in Golden, Colorado. NREL was built to emphasize renewable energy technologies such as photovoltaics and other means of exploiting solar energy. The Materials Sciences and Engineering subprogram supports basic research efforts that underpin this technological emphasis at the Laboratory, for example on overcoming semiconductor doping limits, novel and ordered semiconductor alloys, theoretical and experimental studies of properties of advanced semiconductor alloys for prototype solar cells. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports research addressing the fundamental understanding of solid-state, artificial photosynthetic systems. This research includes the preparation and study of novel dye-sensitized semiconductor electrodes, characterization of

the photophysical and chemical properties of quantum dots, and study of charge carrier dynamics in semiconductors.

## **Oak Ridge Institute for Science and Education**

Oak Ridge Institute for Science and Education (ORISE) is located on 150 acres in Oak Ridge, Tennessee. The BES program provides funding to ORISE for support of a consortium of university and industry scientists to share the ORNL research station at NSLS to study the atomic and molecular structure of matter (known as ORSOAR, the Oak Ridge Synchrotron Organization for Advanced Research). The BES program also funds ORISE to provide administrative support for panel reviews and site reviews commissioned and led by the BES program staff. ORISE also assists with the administration of topical scientific workshops and provides administrative support for other activities such as for the reviews of BES construction projects. ORISE manages the **Shared Research Equipment (SHaRE)** program at ORNL. The SHaRE program makes available state-of-the-art electron beam microcharacterization facilities for collaboration with researchers from universities, industry and other government laboratories.

## **Oak Ridge National Laboratory**

Oak Ridge National Laboratory (ORNL) is a Multiprogram Laboratory located on 24,000 acres in Oak Ridge, Tennessee. ORNL is home to major research efforts in materials and chemical sciences with additional programs in engineering and geosciences. It is the site of the High Flux Isotope Reactor (HFIR) and the Radiochemical Engineering Development Center (REDC). ORNL also leads the six-laboratory collaboration that is designing and constructing the Spallation Neutron Source (SNS).

ORNL has perhaps the most comprehensive materials research program in the country. The Materials Sciences and Engineering subprogram supports basic research that underpins technological efforts such as those supported by the energy efficiency program. Research is conducted in microscopy and microanalysis, atomistic mechanisms in interface science, theoretical studies of metals, alloys, and ceramics, theory and design of dual phase alloys, radiation effects, domain structure in epitaxial ferroelectrics, semiconductor nanocrystals for carbon dioxide fixation, high temperature alloy design, welding science, microstructural design of advanced ceramics, acoustic harmonic generation, non-equilibrium processes. Research is also conducted in superconductivity, magnetic materials, neutron scattering and x-ray scattering, electron microscopy, pulsed laser ablation, thin films, lithium battery materials, thermoelectric materials, surfaces, polymers, structural ceramics, alloys; and intermetallics. The subprogram emphasizes experiments at HFIR and other specialized research facilities that include the High Temperature Materials Laboratory, the Shared Research Equipment (SHaRE) program, and the Surface Modification and Characterization (SMAC) facility. The SMAC facility is equipped with ion implantation accelerators that can be used to change the physical, electrical, and chemical properties of solids to create unique new materials not possible with conventional processing techniques. Surface modification research has led to important practical applications of materials with improved friction, wear, catalytic, corrosion, and other properties. Engineering research provides support for computational nonlinear sciences.

The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports research in analytical chemistry, particularly in the area of mass spectrometry, separation chemistry, and thermo-physical properties. Examples of the science include solvation in supercritical fluids, electric field-assisted separations, speciation of actinide elements, ion-imprinted sol-gels for actinide separations, ligand design, stability of macromolecules and ion fragmentation, imaging of organic and biological materials with secondary ion mass spectrometry, and the physics of highly charged species. The subprogram also supports research on the collision physics of highly charged ions and their interactions with surfaces. In the area of geosciences, work is supported to study low-temperature geochemical processes and rates in mineral-fluid systems.

The **High Flux Isotope Reactor** is a light-water cooled and moderated reactor that began full-power operations in 1966. HFIR operates at 85 megawatts to provide state-of-the-art facilities for neutron scattering, materials irradiation, and neutron activation analysis and is the world's leading source of elements heavier than plutonium for research, medicine, and industrial applications. The neutron-scattering experiments at HFIR reveal the structure and dynamics of a very wide range of materials. The neutron-scattering instruments installed on the four horizontal beam tubes are used in fundamental studies of materials of interest to solid-state physicists, chemists, biologists, polymer scientists, metallurgists, and colloid scientists. Recently, a number of improvements at HFIR have increased its neutron scattering capabilities to 14 state-of-the-art neutron scattering instruments on the world's brightest beams of steady-state neutrons. These upgrades include the installation of larger beam tubes and shutters, a high-performance liquid hydrogen cold source, and neutron scattering instrumentation. The new installation of the cold source provides beams of cold neutrons for scattering research that are as bright as any in the world. Use of these forefront instruments by researchers from universities, industries, and government laboratories are granted on the basis of scientific merit.

The **Radiochemical Engineering Development Center**, located adjacent to HFIR, provides unique capabilities for the processing, separation, and purification of transplutonium elements.

The **Center for Nanophase Materials Sciences (CNMS)**, a proposed BES Nanoscale Science Research Center construction project, will establish a research center and user facility that will integrate nanoscale science research with neutron science, synthesis science, and theory/modeling/simulation. A new building will provide state-of-the-art clean rooms, general laboratories, wet and dry laboratories for sample preparation, fabrication and analysis. Included will be equipment to synthesize, manipulate, and characterize nanoscale materials and structures. The facility, which will be collocated with the Spallation Neutron Source complex, will house over 100 research scientists and an additional 100 students and postdoctoral fellows. The CNMS's major scientific thrusts will be in nano-dimensioned soft materials, complex nanophase materials systems, and the crosscutting areas of interfaces and reduced dimensionality that become scientifically critical on the nanoscale. A major focus of the CNMS will be to exploit ORNL's unique capabilities in neutron scattering to determine the structure of nanomaterials, to develop a detailed understanding of synthesis and self-assembly processes in "soft" materials, and to study and understand collective (cooperative) phenomena that emerge on the nanoscale.

## **Pacific Northwest National Laboratory**

Pacific Northwest National Laboratory (PNNL) is a Multiprogram Laboratory located on 640 acres at the Department's Hanford site in Richland, Washington. The BES Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports research in interfacial chemistry of water-oxide systems, near-field optical microscopy of single molecules on surfaces, inorganic molecular clusters, and direct photon and/or electron excitation of surfaces and surface species. Programs in analytical chemistry and in applications of theoretical chemistry to understanding surface catalysis are also supported. Included among these studies are high-resolution laser spectroscopy for analysis of trace metals on ultra small samples; understanding of the fundamental inter- and intra-molecular effects unique to solvation in supercritical fluids; and interfacing theoretical chemistry with experimental methods to address complex questions in catalysis. Geosciences research includes theoretical and experimental studies to improve our understanding of phase change phenomena in microchannels. The Materials Sciences and Engineering subprogram supports research on molecularly tailored nanostructured materials, stress corrosion and corrosion fatigue, interfacial dynamics during heterogeneous deformation, irradiation assisted stress corrosion cracking, bulk defect and defect processing in ceramics, chemistry and physics of ceramic surfaces and interfacial deformation mechanisms in aluminum alloys.

## **Sandia National Laboratory**

Sandia National Laboratory (SNL) is a Multiprogram Laboratory located on 3,700 acres in Albuquerque, New Mexico (SNL/NM), with sites in Livermore, California (SNL/CA), and Tonopah, Nevada. SNL is home to significant research efforts in materials and chemical sciences with additional programs in engineering and geosciences. SNL/CA is also the site of the Combustion Research Facility (CRF). SNL has a historic emphasis on electronic components needed for Defense Programs. The laboratory has very modern facilities in which unusual microcircuits and structures can be fabricated out of various semiconductors. The Materials Sciences and Engineering subprogram supports projects on the physics and chemistry of ceramics, adhesion and interfacial wetting, localized corrosion initiation, long range particle interactions and collections phenomena in plasma and colloidal crystals, advanced epitaxial growth techniques, energetic particle synthesis, artificially structured semiconductors, field structured anisotropic composites, surface interface and bulk properties of advanced ceramics, transitions in the strongly collective behavior of dislocations, and mixtures of particles in liquids. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram supports geosciences research on mineral-fluid reactivity, rock mechanics, reactive fluid flow and particulate flow through fractured and porous media, and seismic and electromagnetic imaging and inversion studies.

The **Combustion Research Facility** at SNL/CA is an internationally recognized facility for the study of combustion science and technology. In-house efforts combine theory, modeling, and experiment including diagnostic development, kinetics, and dynamics. Several innovative non-intrusive optical diagnostics such as degenerate four-wave mixing, cavity ring-down spectroscopies, high resolution optical spectroscopy, and ion-imaging techniques have been developed to characterize combustion intermediates. Basic research supported by the Chemical Sciences, Geosciences, and Energy Biosciences subprogram is often done in close collaboration with applied problems. A principal effort in turbulent combustion is coordinated among the BES chemical physics program, the Office of Fossil Energy, and the Office of Energy Efficiency and Renewable Energy.

The **Center for Integrated Nanotechnologies (CINT)**, a planned BES Nanoscale Science Research Center, will focus on exploring the path from scientific discovery to the integration of nanostructures into the micro- and macroworlds. This path involves experimental and theoretical exploration of behavior, understanding new performance regimes and concepts, testing designs, and integrating nanoscale materials and structures. CINT focus areas are nanophotonics and nanoelectronics, complex functional nanomaterials, nanomechanics, and the nanoscale/bio/microscale interfaces. CINT will be jointly administered by Los Alamos National Laboratory and Sandia National Laboratory. This Center will make use of a wide range of specialized facilities including the Los Alamos Neutron Science Center and the National High Magnetic Field Laboratory at LANL.

### **Stanford Linear Accelerator Center**

Stanford Linear Accelerator Center (SLAC) is a program-dedicated laboratory (High Energy Physics) located on 426 acres in Menlo Park, California. It is the home of the **Stanford Synchrotron Radiation Laboratory (SSRL)** and peer-reviewed research projects associated with SSRL. The Stanford Synchrotron Radiation Laboratory was built in 1974 to take and use for synchrotron studies the intense x-ray beams from the SPEAR storage ring that was built for particle physics by the SLAC laboratory. Over the years, the SSRL grew to be one of the main innovators in the production and use of synchrotron radiation with the development of wigglers and undulators that form the basis of all third-generation synchrotron sources. In FY 2000, the facility was comprised of 32 experimental stations and was used by nearly 900 researchers from industry, government laboratories and universities. These include astronomers, biologists, chemical engineers, chemists, electrical engineers, environmental scientists, geologists, materials scientists, and physicists. The Materials Sciences and Engineering subprogram supports a research program at SSRL with emphasis in both the x-ray and ultraviolet regions of the spectrum. SSRL scientists are experts in photoemission studies of high-temperature superconductors and in x-ray scattering. The SPEAR 3 upgrade at SSRL will provide major improvements that will increase the brightness of the ring for all experimental stations.

The **Linac Coherent Light Source (LCLS)** will provide laser-like radiation in the x-ray region of the spectrum that is 10 orders of magnitude (i.e., a factor of 10,000,000,000) greater in peak power and peak brightness than any existing coherent x-ray light source. The SLAC linac will provide high-current, low-emittance 5–15 GeV electron bunches at a 120 Hz repetition rate. A newly constructed long undulator will bunch the electrons, leading to self-amplification of the emitted x-ray radiation, constituting the x-ray FEL. The availability of the SLAC linac for the LCLS Project creates a unique opportunity (worldwide) for demonstration and use of x-ray FEL radiation.

### **All Other Sites**

The BES program funds research at 172 colleges/universities located in 49 states. Also included are funds for research awaiting distribution pending completion of peer review results.



# Materials Sciences and Engineering

## Mission Supporting Goals and Objectives

The Materials Sciences and Engineering subprogram delivers the scientific knowledge and discoveries in the materials sciences and engineering that underpin DOE's missions in science, energy, environmental quality, and national security; extends the frontiers of condensed matter physics, metal and ceramic sciences, and materials chemistry, and materials engineering in order to expand the scientific foundations for the development of materials that improve the efficiency, economy, environmental acceptability, and safety in energy generation, conversion, transmission, and use; and plans, constructs, and operates major scientific user facilities to serve researchers at universities, national laboratories, and industrial laboratories.

**The Materials Sciences and Engineering subprogram** supports basic research in condensed matter physics, metal and ceramic sciences, materials chemistry, and materials engineering. This research seeks to understand the atomistic basis of materials properties and behavior and how to make materials perform better at acceptable cost through new methods of synthesis and processing. Basic research is supported in magnetic materials, semiconductors, superconductors, metals, ceramics, alloys, polymers, metallic glasses, ceramic matrix composites, catalytic materials, surface science, corrosion, neutron and x-ray scattering, chemical and physical properties, welding and joining, non-destructive evaluation, electron beam microcharacterization, nanotechnology and microsystems, fluid dynamics and heat transfer in materials, nonlinear systems, and new instrumentation. Ultimately the research leads to the development of materials that improve the efficiency, economy, environmental acceptability, and safety in energy generation, conversion, transmission, and use. For example, the fuel economy in automobiles is directly proportional to the weight of the automobile, and fundamental research on strength of materials has led to stronger, lighter materials, which directly affects fuel economy. The efficiency of a combustion engine is limited by the temperature and strength of materials, and fundamental research on alloys and ceramics has led to the development of materials that retain their strength at high temperatures. Research in semiconductor physics has led to substantial increases in the efficiency of photovoltaic materials for solar energy conversion. Fundamental research in condensed matter physics and ceramics has underpinned the development of practical high-temperature superconducting wires for more efficient transmission of electric power. This subprogram is a premier sponsor of condensed matter and materials physics in the U.S., is the primary supporter of the BES user facilities, and is responsible for the construction of the Spallation Neutron Source. **Performance will be measured by** reporting accomplishments on the common performance measures on leadership, excellence, and relevance; quality; and safety and health.

## Funding Schedule

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
Materials Sciences and Engineering Research.....	228,141	236,842	261,028	+24,186	+10.2%
Facilities Operations .....	283,467	263,865	274,118	+10,253	+3.9%
SBIR/STTR .....	0	11,815	12,737	+922	+7.8%
<b>Total, Materials Sciences and Engineering..</b>	<b>511,608</b>	<b>512,522</b>	<b>547,883</b>	<b>+35,361</b>	<b>+6.9%</b>

## Detailed Program Justification

(dollars in thousands)

	FY 2001	FY 2002	FY 2003
<b>Materials Sciences and Engineering Research .....</b>	<b>228,141</b>	<b>236,842</b>	<b>261,028</b>
▪ <b>Structure and Composition of Materials .....</b>	<b>33,767</b>	<b>36,070</b>	<b>36,697</b>

This activity supports basic research in the structure and characterization of materials; the relationship of structure to the behavior and performance of materials; predictive theory and modeling; and new materials such as bulk metallic glasses and nanophase materials. This activity also supports four electron beam microcharacterization user centers: the Center for Microanalysis of Materials at the University of Illinois, the Electron Microscopy Center for Materials Research at Argonne National Laboratory, the National Center for Electron Microscopy at Lawrence Berkeley National Laboratory, and the Shared Research Equipment Program at Oak Ridge National Laboratory. These network-interfaced centers contain a variety of highly specialized instruments to characterize localized atomic positions and configurations, chemical gradients, interatomic bonding forces, etc.

The properties and performance of materials used in all areas of energy technology depend upon their structure. Performance improvements for environmentally acceptable energy generation, transmission, storage, and conversion technologies likewise depend upon the structural characteristics of advanced materials. This dependency occurs because the spatial and chemical inhomogeneities in materials (e.g. dislocations, grain boundaries, magnetic domain walls and precipitates, etc.) determine and control critical behaviors such as fracture toughness, ease of fabrication by deformation processing, charge transport and storage capacity, superconducting parameters, magnetic behavior, and corrosion susceptibility, etc.

In FY 2003, major activities will be responsive to the need for advanced instruments with capabilities to characterize and interpret atomic configurations and packing arrangements at the nanoscale with improved resolution and accuracy, including the ability to determine composition, bonding, and physical properties of materials. Many of these advanced tools will come from the further development of current microscopies; however, new instruments are needed as well. Additional funding is requested to address one of the major recommendations of BESAC following its FY 2000 review of the electron beam microcharacterization centers for the design of components for an aberration corrected transmission electron microscope. This instrument would advance understanding in many areas related to energy mission needs such as interfaces in solid-state devices, load-bearing

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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structural composites and protective coatings; deformation behavior that relates to the processing of metals; grain boundary sliding that degrades the strength of structural alloys and ceramics at elevated temperatures; domain walls in ferromagnetic and ferroelectric materials; vortices and flux pinning in superconductors; and long-standing problems of brittle fracture and fracture resistance. Additional funding is also requested to address another BESAC recommendation to enhance the remote telepresence operations at the electron beam microcharacterization centers.

Capital equipment is provided for items such as new electron microscopes and improvements to existing instruments.

▪ **Mechanical Behavior and Radiation Effects** ..... **15,286**    **14,530**    **14,530**

This activity supports basic research to understand the mechanical behavior of materials under static and dynamic stresses and the effects of radiation on materials properties. The objective is to understand at the atomic level the relationship between mechanical properties and defects in materials, including defect formation, growth, migration, and propagation. In the area of mechanical behavior, the research aims to build on this atomic level understanding in order to develop predictive models for the design of materials having prescribed mechanical behavior, with some emphasis on very high temperatures. In the areas of radiation effects, the research aims to advance atomic level understanding of amorphization mechanisms (transition from crystalline to a non-crystalline phase) to predict and suppress radiation damage, develop radiation-tolerant materials, and modify surfaces by such techniques as ion implantation.

This program contributes to DOE missions in the areas of fossil energy, fusion energy, nuclear energy, transportation systems, industrial technologies, defense programs, radioactive waste storage, energy efficiency, and environment management. This research helps understand load-bearing capability, failure and fatigue resistance, fracture toughness and impact resistance, high-temperature strength and dimensional stability, ductility or deformability of materials that is critical to their ease of fabrication, and radiation effects including understanding and modeling of radiation damage and surface modification using ion implantation. This activity relates to energy production and conversion through the need for failure resistant materials that perform reliably in the hostile and demanding environments of energy production and use. In an age when economics require life extension of materials and environmental and safety concerns demand reliability, the ability to predict performance from a fundamental basis is a priority. Furthermore, high energy-conversion efficiency requires materials that maintain their structural integrity at high operating temperatures. This program contributes to understanding of mechanical properties of materials and aspects of nuclear technologies ranging from radioactive waste storage to extending the lifetime of nuclear facilities.

In FY 2003, major activities will include continued development of experimental techniques and methods for the characterization of mechanical behavior, the development of a universal model for mechanical behavior that includes all length scales from atomic to nanoscale to bulk dimensions, and advancement of computer simulations for modeling behavior and radiation induced degradation.

Capital equipment is provided for items such as in-situ high-temperature furnaces, and characterization instrumentation.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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▪ **Physical Behavior of Materials**..... **16,449**    **15,735**    **15,735**

This activity supports basic research at the atomic and molecular level to understand, predict, and control physical behavior of materials by developing rigorous models for the response of materials to environmental stimuli such as temperature, electromagnetic field, chemical environment, and proximity of surfaces or interfaces. Included within the activity are research in aqueous, galvanic, and high-temperature gaseous corrosion and their prevention; photovoltaics and photovoltaic junctions and interfaces for solar energy conversion; the relationship of crystal defects to the superconducting properties for high-temperature superconductors; phase equilibria and kinetics of reactions in materials in hostile environments, such as in the very high temperatures encountered in energy conversion processes; diffusion and the transport of ions in ceramic electrolytes for improved performance batteries and fuel cells.

Research underpins the mission of DOE by developing the basic science necessary for improving the reliability of materials in mechanical and electrical applications and for improving the generation and storage of energy. With increased demands being placed on materials in real-world environments (extreme temperatures, strong magnetic fields, hostile chemical environments, etc), understanding how their behavior is linked to their surroundings and treatment history is critical.

In FY 2003, major activities will continue fundamental studies of corrosion resistance and surface degradation; semiconductor performance; high-temperature superconductors; and the interactions, and transport of defects in crystalline matter.

Capital equipment is provided for items such as spectroscopic instruments, instruments for electronic and magnetic property measurement, and analytical instruments for chemical and electrochemical analysis.

▪ **Synthesis and Processing Science** ..... **12,801**    **14,690**    **18,595**

This activity supports basic research on understanding and developing innovative ways to make materials with desired structure, properties, or behavior. Examples include materials synthesis and processing to achieve new or improved behavior, for minimization of waste, and for hard and wear resistant surfaces; high-rate, superplastic forming of light-weight metallic alloys for fuel efficient vehicles; high-temperature structural ceramics and ceramic matrix composites for high-speed cutting tools and fuel efficient and low-pollutant engines; non-destructive analysis for early warning of impending failure and flaw detection during production; response of magnetic materials to applied static and cyclical stress; plasma, laser, charged particle beam surface modification to increase corrosion resistance; and processing of high-temperature, intermetallic alloys.

The activity includes the operation of the Materials Preparation Center at the Ames Laboratory, which develops innovative and superior processes for materials preparation and provides small quantities of unique, research-grade materials that are not otherwise available to academic, governmental, and industrial research communities.

These activities underpin many of the DOE technology programs, and appropriate linkages have been established in the areas of light-weight, metallic alloys; structural ceramics; high-temperature superconductors; and industrial materials, such as intermetallic alloys.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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In FY 2003, new funding is requested for new research on nanoscale synthesis and processing. The mechanical properties of materials change dramatically as the grain size in polycrystalline materials approaches the nanometer scale. At conventional grain sizes a gain in strength of a material typically results in a loss in both ductility and fracture toughness resulting in a brittle material; however, by using nanocomposites and understanding deformation physics, we should be able to make materials that are both strong, tough (resistant to impact fracture) and ductile. The classical law for predicting the dependence of mechanical strength on particle, crystal or grain size appears to break down in the size regime of about 10 to 100 nanometers. A fundamental understanding of both deformation and embrittlement will require new tools, including massively parallel processing computers, techniques for establishing activation energies from atomistic calculations, methods for simplifying computations involving dislocation configurations and networks, electron microscopy, and direct, real-time dislocation studies (densities, types, and patterning). Deformation and fracture are very important to DOE. Embrittlement is a major cause of catastrophic failure in materials. Plastic deformation, which requires ductility, is used for almost all fabrication of structural metals (rolling, spinning, forging, extruding, and drawing); and plastic deformation can also change critical dimensions of materials in energy systems exposed to high temperatures, mechanical loads, or irradiation. Scientific and technological breakthroughs in materials research and development are very often directly coupled to progress in synthesis and processing. A way to control the size, size distribution and assembly of nanoparticles is to use patterns on surfaces. If successful, these assemblies could be used for solar energy conversion, efficient lighting, very sensitive sensors, nanoelectronic devices, improved corrosion and wear resistance and very high-density magnetic information storage. There is also great need for nanoparticles of uniform size, composition, and surface stability because experiments have shown that fracture toughness may undergo a profound increase as the grain size falls below 10 to 50 nm in high-temperature structural ceramics. These materials might be used in advanced fuel efficient engines, turbines, and machine cutting tools

Capital equipment includes furnaces, lasers, processing equipment, plasma and ion sources, and deposition equipment.

▪ **Engineering Research**..... **17,352**    **16,480**    **16,480**

This activity focuses on nanotechnology and microsystems; multi-component fluid dynamics and heat transfer; and non-linear dynamic systems. In the area of nanoscience, work focuses on nanomechanics and nano to micro assembly, networks of nano sensors, hybrid microdevices, energy transport and conversion, nanobioengineering, nucleation and nanoparticle engineering issues.

In FY 2003, efforts will continue in select topics of nano-engineering; predictive non-destructive evaluation of structures coupled with micromechanics and nano/microtechnology; multi-phase flow and heat transfer; system sciences, control, and instrumentation; and data and engineering analysis.

▪ **Neutron and X-ray Scattering** ..... **31,682**    **40,611**    **54,377**

This activity supports basic research in condensed matter physics and materials physics using neutron and x-ray scattering capabilities, primarily at major BES-supported user facilities. Research seeks to achieve a fundamental understanding of the atomic, electronic, and magnetic structures of materials as well as the relationship of these structures and excitations to the physical properties of materials. The

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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increasing complexity of such energy-relevant materials as superconductors, semiconductors, and magnets requires ever more sophisticated neutron and x-ray scattering techniques to extract useful knowledge and develop new theories for the behavior of these materials. Both ordered and disordered materials are of interest as are strongly correlated electron systems, surface and interface phenomena, and behavior under environmental variables such as temperature, pressure, and magnetic field. Neutron and x-ray scattering, together with the electron scattering probes supported under Structure and Composition of Materials, are the primary tools for characterizing the atomic, electronic and magnetic structures of materials.

Included within this request are funds to increase x-ray and neutron science activities in the U.S. based on BES reviews of the synchrotron radiation light sources, on discussions within the OSTP Interagency Working Group on Neutron Science, and on three BESAC reviews that addressed the current status of research activities using neutron scattering in the U.S. and strategies needed to take full advantage of the SNS upon its completion. Funding is increased for new and upgraded instrumentation to take advantage of scientific opportunities in the physical sciences and to leverage the multibillion-dollar investment in these facilities. Funds will be competed among both laboratory and academic institutions for multiyear beamline and instrument development projects in the range \$5,000,000-15,000,000 each in such areas as materials sciences, surface science, condensed matter physics, atomic and molecular physics, polymers and soft materials, nanostructured materials, x-ray microscopy, tomography, femtosecond phenomena, interfacial studies, and imaging. Of these funds, \$5,000,000 is provided for the development of instrumentation to exploit the scientific potential of the SNS facility. These instruments will be built by individual DOE laboratories or consortia of DOE laboratories and the SNS based on scientific merit and importance to users from universities, industries, and government laboratories. Funding is also increased for academic scientists to participate in the development of neutron scattering instruments and for the neutron science/scattering programs at the host institutions of the BES facilities, where historically the interplay between science programs and instrument design and fabrication has produced advances in instrumentation and seminal scientific results.

Capital equipment is provided for items such as detectors, monochromators, mirrors, and beamline instrumentation at all of the facilities.

▪ **Experimental Condensed Matter Physics ..... 35,837 34,115 38,020**

This activity supports a broad-based experimental program in condensed matter and materials physics with selected emphasis in the areas of electronic structure, surfaces/interfaces, and new materials. Research includes measurements of the properties of solids, liquids, glasses, surfaces, thin films, artificially structured materials, self-organized structures, and nanoscale structures. The materials examined include magnetic materials, superconductors, semiconductors and photovoltaics, liquid metals and alloys, and complex fluids. The development of new techniques and instruments including magnetic force microscopy, electron microscopic techniques, and innovative applications of laser spectroscopy is a major component of this activity. Measurements will be made under extreme conditions of temperature, pressure, and magnetic field - especially with the availability of the 100 Tesla pulsed field magnet at LANL.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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This research is aimed at a fundamental understanding of the behavior of materials that underpin DOE technologies. Presently, the portfolio includes specific research thrusts in magnetism, semiconductors, superconductivity, materials synthesis and crystal growth, and photoemission spectroscopy. The portfolio addresses well-recognized needs, including understanding magnetism and superconductivity; the control of electrons and photons in solids; understanding materials at reduced dimensionality; the physical properties of large, interacting systems; and the properties of materials under extreme conditions.

The combined projects in superconductivity comprise a concerted and comprehensive energy-related research program. The DOE laboratories anchor the BES multi-disciplinary basic research efforts and maintain integration with the Energy Efficiency (EE) program applied and developmental efforts. Research on magnetism and magnetic materials focuses on hard magnet materials, such as those used for permanent magnets and in motors. This activity provides direct research assistance to the technology programs in Energy Efficiency and Renewable Energy (EE/RW) (photovoltaics, superconductivity, power sources), (thermoacoustics), and in National Nuclear Security Administration (NNSA) (photoemission, positron research, and electronic and optical materials). In addition, it supports, more fundamentally, several DOE technologies and the strategically important information technology and electronics industries through its results in the fields of semiconductor physics, ion implantation and electronics research; the petroleum recovery efforts of Fossil Energy and the clean-up efforts of Environmental Management (EM) programs through research on granular materials and on fluids; through EE research on advanced materials and magnets; energy conservation efforts through research on ion implantation, ultra-hard materials, superconductivity, thermoelectrics, and power source component materials; and NNSA through research on advanced laser crystals and weapons-related materials.

In FY 2003, new funding is requested for increased effort in experimental condensed matter physics to answer very fundamental questions in condensed matter physics at the nanoscale. As the size of a nanoscale structure becomes less than the average length for scattering of electrons or phonons, new modes of transport for electrical current and/or heat become possible. Also thermodynamic properties, including collective phenomena and phase transitions such as ferromagnetism, ferroelectricity, and superconductivity can change when structures contain a small number of atoms. The potential impacts of understanding the physics are very significant. For example, nanoscale structures provide a path toward the next generation of powerful permanent magnets for more efficient electric motors, better thermoelectric materials, and materials for more efficient solar energy conversion. In the case of soft materials, the physics of association and configuration of large molecules is poorly understood. Yet this kind of self assembly, which ubiquitous in nature, will be required for many of the potential applications of nanoscale science. Even the most rudimentary steps, such as how a macromolecule finds its equilibrium shape, are still in controversy. Much less is known about how such molecules can assemble into larger structures with defined shapes. Self-assembled macromolecules can provide very strong, lightweight materials that would decrease the weight in automobiles improving fuel economy.

Capital equipment is provided for crystal growth equipment, scanning tunneling microscopes, electron detectors for photoemission experiments, sample chambers, superconducting magnets and computers.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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▪ **Condensed Matter Theory** ..... **16,124**    **18,007**    **18,007**

This activity supports basic research in theory, modeling, and simulations, and it complements the experimental work. The links between the electronic, optical, mechanical, and magnetic properties of nanostructures and their size, shape, topology, and composition are not well understood. For the simplest semiconductor systems, carbon nanotubes, and similar “elementary” systems, there has been considerable progress. However, for more complex materials and hybrid structures, even the outlines of a theory remain to be made. Computer simulations will play a major role in understanding materials at the nanometer scale and in the development “by design” of new nanoscale materials and devices. The greatest challenges and opportunities are in the transition regions where nanoscale phenomena are just beginning to emerge from the macroscopic and microscale regimes, which may be described by bulk properties plus the effects of interfaces and lattice defects.

This activity also supports the Center for X-ray Optics at LBNL, the Center for Advanced Materials at LBNL, the Surface Modification and Characterization Facility at ORNL, and the Center for Synthesis and Processing of Advanced Materials, which consists of collaborating projects at national laboratories, universities, and industry.

In FY 2003, this activity will provide support for theory, modeling and large-scale computer simulation to explore new nanoscale phenomena and the nanoscale regime. Also supported is the Computational Materials Sciences Network for studies of such topics as polymers at interfaces; fracture mechanics - understanding ductile and brittle behavior; microstructural evolution and microstructural effects on mechanics of materials, magnetic materials, modeling oxidation processes at surfaces and interfaces, and excited state electronic structure and response functions.

Capital equipment is provided for items such as computer workstations, beamline instruments, ion implantation and analytical instruments.

▪ **Materials Chemistry** ..... **30,808**    **27,650**    **29,602**

This activity supports basic research on the chemical properties of materials to understand the effect of chemical reactivity on the behavior of materials and to synthesize new chemical compounds and structures from which better materials can be made. Research topics supported include solid state chemistry, surface chemistry, polymer chemistry, crystallography, synthetic chemistry, and colloid chemistry. Also supported are investigations of novel materials such as low-dimensional, self-assembled monolayers; polymeric conductors; organic superconductors and magnets; complex fluids; and biomolecular materials. The research employs a wide variety of experimental techniques to characterize these materials, including x-ray photoemission and other spectroscopies, scanning tunneling and atomic force microscopies, nuclear magnetic resonance, and x-ray and neutron reflectometry. The activity also supports the development of new experimental techniques, such as high-resolution magnetic resonance imaging without magnets, neutron reflectometry, and atomic force microscopy of liquids.

The research underpins many technological areas, such as batteries and fuel cells, catalysis, friction and lubrication, membranes, electronics, and environmental chemistry. New techniques for fabrication of nanocrystals, such as a unique inverse micellar process, make possible the efficient elimination of



(dollars in thousands)

FY 2001	FY 2002	FY 2003
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dangerous chlorinated organic and phenolic pollutants (e.g., PCPs). Research on solid electrolytes has led to very thin rechargeable batteries that can be recharged many more times than existing commercial cells. Research on chemical vapor deposition (CVD) continues to impact the electronics industry. The development of synthetic membranes using biological synthesis may yield materials for separations and energy storage, and research on polymers may lead to light-weight structural materials which can be used in automobiles and thereby providing substantial savings in energy efficiency.

In FY 2003, work will continue on the systematic and parallel patterning of matter on the nanometer scale. There are many powerful approaches to patterning on the nanoscale that are fundamentally serial in nature, for instance, atom manipulation using scanning probe tips or electron beam lithography. The research in this activity will focus on methods to prepare macroscopic quantities of nanoscale components in complex, designed patterns, using techniques of self assembly. An increase is requested for research to understand how the shapes of molecular building blocks affect the spontaneous assembly into fibers, membranes, and other large-scale structures and to understand the effects of pressure, ionic strength, solvents, and external electric and magnetic fields on the shape and properties of the large-scale structures. This work on self-controlling materials lies at the interface of the physical sciences, molecular biology, and materials engineering. Both natural and synthetic molecules in combination can be used to make new molecular species, and the techniques of molecular self-assembly can be used to create new structures with new properties on the nanoscale. This work will focus on the study of simple structures and phenomena and on the emerging arsenal of tools and techniques such as combinatorial chemistry needed to explore the properties and structures of these new materials.

Capital equipment is provided for such items as chambers to synthesize and grow new materials, nuclear magnetic resonance and electron spin resonance spectrometers, lasers, neutron reflectometers, x-ray beamlines, and atomic force microscopes.

▪ **Experimental Program to Stimulate Competitive Research.....**                    **7,685**            **7,679**            **7,685**

This activity supports basic research spanning the complete range of activities within the Department in states that have historically received relatively less Federal research funding. The EPSCoR states are Alabama, Alaska, Arkansas, Hawaii, Idaho, Kansas, Kentucky, Louisiana, Maine, Mississippi, Montana, Nebraska, Nevada, New Mexico, North Dakota, Oklahoma, South Carolina, South Dakota, Vermont, West Virginia, and Wyoming, and the Commonwealth of Puerto Rico. The work supported by the EPSCoR program includes research in materials sciences, chemical sciences, biological and environmental sciences, high energy and nuclear physics, fusion energy sciences, fossil energy sciences, and energy efficiency and renewable energy sciences.

## EPSCoR Distribution of Funds by State

(dollars in thousands)

	FY 2001	FY 2002 Estimate	FY 2003 Estimate
Alabama .....	350	375	375
Alaska <sup>a</sup> .....	0	0	0
Arkansas.....	115	65	65
Hawaii <sup>b</sup> .....	0	0	0
Idaho.....	107	60	60
Kansas.....	933	615	615
Kentucky.....	468	471	471
Louisiana .....	130	130	130
Maine.....	0	0	0
Mississippi .....	652	535	535
Montana.....	515	465	465
Nebraska .....	480	300	300
Nevada .....	614	325	325
New Mexico <sup>b</sup> .....	0	0	0
North Dakota .....	0	55	55
Oklahoma .....	165	65	65
Puerto Rico.....	450	435	435
South Carolina.....	1,201	120	120
South Dakota.....	0	0	0
Vermont .....	585	585	585
West Virginia.....	794	525	525
Wyoming.....	59	65	65
Technical Support.....	67	400	400
Other.....	0	2,088 <sup>c</sup>	2,094 <sup>c</sup>
<b>Total .....</b>	<b>7,685</b>	<b>7,679</b>	<b>7,685</b>

<sup>a</sup> Alaska becomes eligible for funding in FY 2001.

<sup>b</sup> Hawaii and New Mexico become eligible for funding in FY 2002.

<sup>c</sup> Uncommitted funds in FY 2002 and FY 2003 will be competed among all EPSCoR states.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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- **Extension of HB-2 Beam Tube at the High Flux Isotope Reactor** ..... **1,150**      **0**      **0**

This project is a major item of equipment with a total estimated cost of \$5,550,000 that provided beam access for six thermal neutron scattering instruments. The project was completed in FY 2001.
- **Neutron Scattering Instrumentation at the High Flux Isotope Reactor** ..... **0**      **2,000**      **2,000**

Capital equipment funds are provided for new and upgraded instrumentation, such as spectrometers, diffractometers, and detectors.
- **SPEAR3 Upgrade** ..... **8,300**      **8,300**      **9,300**

Over the period FY 1999 - FY 2003, the SPEAR3 upgrade (funded in both BES subprograms) is being undertaken at SSRL to provide major improvements to all existing experimental stations served by this synchrotron radiation light source. The technical goals are to increase injection energy from 2.3 GeV to 3 GeV to improve the energy spectrum available to users; decrease beam emittance by a factor of 7 to increase beam brightness; increase operating current from 100 mA to 200 mA to increase beam intensity; and maintain long beam life time (>25 hr). The increased photon flux will greatly improve performance in a variety of applications including powder and thin film diffraction, topographic studies, surface microcontamination studies, x-ray tomographic analysis, x-ray absorption studies, and protein crystallography. The magnets and associated vacuum chambers of the existing SPEAR storage ring will be replaced in order to implement the revised lattice system. All components are housed within the existing buildings. The TEC is \$29,000,000; DOE and NIH are equally funding the upgrade with a total Federal cost of \$58,000,000. NIH has provided \$14,000,000 in FY 1999, \$14,000,000 in FY 2000, and \$1,000,000 in FY 2001. The funding profile, but not the TEC, of this MIE has been modified based on an Office of Science construction project review, which recommended that some funds be shifted from later years to early years in order to reduce schedule risk by ensuring that critical components are available for installation when scheduled. That recommendation was accepted and is reflected in the current funding profile.
- **Advanced Light Source Beamline** ..... **900**      **975**      **0**

This beamline is a major item of equipment with a total estimated cost of \$6,000,000 that will provide capabilities for surface and interfacial science important to geosciences, environmental science, and aqueous corrosion science. It is being funded jointly by the Materials Sciences and Engineering subprogram and the Chemical Sciences, Geosciences, and Energy Biosciences subprogram.

(dollars in thousands)

	FY 2001	FY 2002	FY 2003
<b>Facilities Operations</b> .....	<b>283,467</b>	<b>263,865</b>	<b>274,118</b>
▪ <b>Operation of National User Facilities</b> .....	<b>268,126</b>	<b>263,865</b>	<b>274,118</b>

The facilities included in Materials Sciences and Engineering are: Advanced Light Source, Advanced Photon Source, National Synchrotron Light Source, Stanford Synchrotron Radiation Laboratory, High Flux Isotope Reactor, Intense Pulsed Neutron Source, and Manuel Lujan, Jr. Neutron Scattering Center. Research and development in support of the construction of the Spallation Neutron Source is also included. The Combustion Research Facility is funded in the Chemical Sciences, Geosciences, and Energy Biosciences subprogram. The facility operations budget request, presented in a consolidated manner later in this budget, includes operating funds, capital equipment, and Accelerator and Reactor Improvements (AIP) funding under \$5,000,000. AIP funding will support additions and modifications to accelerator and reactor facilities that are supported in the Materials Sciences and Engineering subprogram. General Plant Project (GPP) funding is also required for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems. The total estimated cost of each GPP project will not exceed \$5,000,000. Capital equipment is needed at the facilities for items such as beam monitors, interlock systems, vacuum systems, beamline front end components, monochromators, and power supplies. A summary of the funding for the facilities included in the Materials Sciences and Engineering subprogram is provided below.

▪ <b>High Flux Beam Reactor (HFBR)</b> .....	<b>15,341</b>	<b>0</b>	<b>0</b>
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The HFBR has been closed. Responsibility for the reactor has been transferred from SC to the Office of Environmental Management (EM) for surveillance and decommissioning. Surveillance will continue until the reactor is fully decommissioned and decontaminated by EM.

(dollars in thousands)

	FY 2001	FY 2002	FY 2003
Facilities			
Advanced Light Source .....	35,605	37,009	39,561
Advanced Photon Source.....	90,314	87,380	91,291
National Synchrotron Light Source.....	34,720	33,671	35,893
Stanford Synchrotron Radiation Laboratory.....	21,696	21,357	22,673
High Flux Beam Reactor .....	15,341	0	0
High Flux Isotope Reactor.....	37,197	37,872	36,854
Radiochemical Engineering Development Center .....	6,512	6,606	6,712
Intense Pulsed Neutron Source.....	13,833	15,826	17,015
Manuel Lujan, Jr. Neutron Scattering Center.....	9,190	9,044	9,678
Spallation Neutron Source.....	19,059	15,100	14,441
Total, Facilities.....	283,467	263,865	274,118

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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**SBIR/STTR**..... **0 11,815 12,737**

In FY 2001, \$9,563,000 and \$574,000 were transferred to the SBIR and STTR programs, respectively. The FY 2002 and FY 2003 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.

**Total, Materials Sciences and Engineering** ..... **511,608 512,522 547,883**

### Explanation of Funding Changes from FY 2002 to FY 2003

FY 2003 vs. FY 2002 (\$000)
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#### Materials Sciences and Engineering Research

- Increase for structure and composition of materials for the design of components for an aberration corrected transmission electron microscope and to enhance remote operations of the electron beam microcharacterization centers..... +627
  - Increase in the area of synthesis and processing for developing a fundamental understanding of nanoscale processes involved in materials deformation and fracture, synthesis of ordered arrays of nanoparticles using patterns techniques and synthesis of nanoparticles of uniform size and shape..... +3,905
  - Increase for neutron and x-ray scattering for new and upgraded instrumentation fabricated both by university and DOE laboratory researchers and for increased support for academic researchers and students. Within this increase, \$5,000,000 is provided for instrumentation for the SNS. .... +13,766
  - Increase in condensed matter physics for understanding how properties change or can be improved at the nanoscale and how macromolecules reach their equilibrium configuration and self assemble into larger structures..... +3,905
  - Increase for materials chemistry for research on self assembly of materials at the atomic/molecular level..... +1,952
  - Increase for the Experimental Program to Stimulate Competitive Research to restore funding to FY 2001 levels..... +6
  - Increase in capital equipment funds for the SPEAR3 MIE per approved profile .... +1,000
  - Decrease in capital equipment funds for the ALS Beamline MIE per approved profile..... -975
- Total, Materials Sciences and Engineering Research..... +24,186

FY 2003 vs. FY 2002 (\$000)
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**Facilities Operations**

▪ Increase for operations for the Advanced Light Source. ....	+2,552
▪ Increase for operations for the Advanced Photon Source.....	+3,911
▪ Increase for operations for the National Synchrotron Light Source.....	+2,222
▪ Increase for operations for the Stanford Synchrotron Radiation Laboratory.....	+1,316
▪ Decrease for operations for the High-Flux Isotope Reactor because of completion of Cold Guide Hall Extension (\$-2,800,000) and increase for HFIR operations (\$+1,782,000) .....	-1,018
▪ Increase for operations for Radiochemical Engineering Development Center .....	+106
▪ Increase for operations for the Intense Pulsed Neutron Source.....	+1,189
▪ Increase for operations for the Manuel Lujan, Jr. Neutron Scattering Center.....	+634
▪ Decrease in the Spallation Neutron Source research and development funds per FY 2002 project datasheet .....	-659
Total, Materials Sciences and Engineering Facilities Operations. ....	+10,253

**SBIR/STTR**

▪ Increase in SBIR/STTR funding because of increase in operating expenses.....	+922
Total Funding Change, Materials Sciences and Engineering.....	+35,361

# Chemical Sciences, Geosciences, and Energy Biosciences

## Mission Supporting Goals and Objectives

The Chemical Sciences, Geosciences, and Energy Biosciences subprogram delivers the scientific knowledge and discoveries in the chemical sciences, geosciences, and biosciences that underpin DOE's missions in science, energy, environmental quality, and national security; extends the frontiers of fundamental chemical interactions and molecular processes in order to expand the scientific foundations for the development of such advances as efficient combustion systems with reduced emissions of pollutants; new solar photoconversion processes; improved catalysts for cleaner, more efficient, and efficient and cheaper production of fuels and chemicals; and better separations and analytical methods for applications in every DOE mission area; extends the frontiers of energy processes, environmental remediation, and waste management; and geochemistry and geophysics to expand the scientific foundations for contaminant remediation, reservoir definition, and fluid transport to predict repository performance; extends the frontiers of biosciences in order to expand the scientific foundations for the development of renewable biomass resources and the light-driven production of chemical energy via natural photosynthesis; plans, constructs, and operates major scientific user facilities to serve researchers at universities, national laboratories, and industrial laboratories.

**The Chemical Sciences, Geosciences, and Energy Biosciences subprogram** supports basic research in atomic, molecular and optical science; chemical physics; photochemistry; radiation chemistry; physical chemistry; inorganic chemistry; organic chemistry; analytical chemistry; separation science; heavy element chemistry, geochemistry, geophysics, and physical biosciences. This research seeks to understand chemical reactivity through studies of the interactions of atoms, molecules, and ions with photons and electrons; the making and breaking of chemical bonds in the gas phase, in solutions, at interfaces, and on surfaces; and energy transfer processes within and between molecules. Ultimately, this research leads to the development of such advances as efficient combustion systems with reduced emissions of pollutants; new solar photoconversion processes; improved catalysts for clean and efficient production of fuels and chemicals; and better separations and analytical methods for applications in energy processes, environmental remediation, and waste management. The geosciences activity supports mineral-fluid interactions; rock, fluid, and fracture physical properties; and new methods and techniques for geosciences imaging from the atomic scale to the kilometer scale. The activity contributes to the solution of problems in multiple DOE mission areas, including reactive fluid flow studies to understand contaminant remediation; seismic imaging for reservoir definition; and coupled hydrologic-thermal-mechanical-reactive transport modeling to predict repository performance. The bioscience activity supports basic research in molecular-level studies on solar energy capture through natural photosynthesis; the mechanisms and regulation of carbon fixation and carbon energy storage; the synthesis, degradation, and molecular interconversions of complex hydrocarbons and carbohydrates; and the study of novel biosystems and their potential for materials synthesis, chemical catalysis, and materials synthesized at the nanoscale. This subprogram provides support for chemistry equal to that of the National Science Foundation. It is the Nation's sole support for heavy-element chemistry, and it is Nation's primary support for homogeneous and heterogeneous catalysis, photochemistry, radiation

chemistry, separations and analysis, and gas-phase chemical dynamics. This subprogram further provides one third of the federal support for individual investigator research in solid earth sciences.

**Performance will be measured** by reporting accomplishments on the common performance measures on leadership, excellence and relevance; quality; and safety and health.

### Funding Schedule

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
Chemical Sciences, Geosciences, and Energy Biosciences Research .....	197,768	197,636	209,319	+11,683	+5.9%
Facilities Operations .....	5,463	5,377	5,805	+428	+8.0%
SBIR/STTR .....	0	4,770	5,022	+252	+5.3%
<b>Total, Chemical Sciences, Geosciences, and Energy Biosciences .....</b>	<b>203,231</b>	<b>207,783</b>	<b>220,146</b>	<b>+12,363</b>	<b>+5.9%</b>

### Detailed Program Justification

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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#### Chemical Sciences, Geosciences, and Energy Biosciences Research .....

**197,768    197,636    209,319**

#### ▪ Atomic, Molecular, and Optical (AMO) Science .....

**11,428    11,815    11,815**

This activity supports theory and experiments to understand the properties of and interactions among atoms, molecules, ions, electrons, and photons. Included among the research activities are studies to determine the quantum mechanical description of such properties and interactions; interactions of intense electromagnetic fields with atoms and molecules; development and application of novel x-ray light sources; and ultracold collisions and quantum condensates. This activity also supports the James R. MacDonald Laboratory at Kansas State University, a multi-investigator program and BES collaborative research center devoted to experimental and theoretical studies of collision processes involving highly charged ions.

The knowledge and techniques developed in this activity have wide applicability. Results of this research provide new ways to use photons, electrons, and ions to probe matter in the gas and condensed phases. This has enhanced our ability to understand materials of all kinds and enables the full exploitation of the BES synchrotron light sources, electron beam micro-characterization centers, and neutron scattering facilities. Furthermore, by studying energy transfer within isolated molecules, AMO science provides the very foundation for understanding chemical reactivity, i.e., the process of energy transfer between molecules and ultimately the making and breaking of chemical bonds.



(dollars in thousands)

FY 2001	FY 2002	FY 2003
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The AMO Science activity is the sole supporter of synchrotron-based AMO science studies in the U.S., which includes ultrashort x-ray pulse generation and utilization at the ALS and APS. This program is also the principal U.S. supporter of research in the properties and interactions of highly charged atomic ions, which are of direct consequence to fusion plasmas.

Research priorities for FY 2003 include the interactions of atoms and molecules with intense electromagnetic fields that are produced by collisions with highly charged ions or short laser pulses; the use of optical fields to control quantum mechanical processes; atomic and molecular interactions at ultracold temperatures and the creation and utilization of quantum condensates, which provides strong linkages between atomic and condensed matter physics at the nanoscale; and the development and application of novel x-ray light sources based on table-top lasers and new utilization of third generation synchrotrons in advance of next-generation BES light sources.

Capital equipment is provided for items including lasers and optical equipment, unique ion sources or traps, position sensitive and solid-state detectors, control and data processing electronics.

▪ **Chemical Physics Research**..... **27,875**      **33,285**      **33,285**

This activity supports experimental and theoretical investigations of gas phase chemistry and chemistry at surfaces. Gas phase chemistry emphasizes the dynamics and rates of chemical reactions at energies characteristic of combustion with the aim of developing validated theories and computational tools for predicting chemical reaction rates for use in combustion models and experimental tools for validating these models. The study of chemistry at well characterized surfaces and the reactions of metal and metal oxide clusters leads to the development of theories on the molecular origins of surface mediated catalysis.

This activity also has oversight for the Combustion Research Facility (which is budgeted below in Facilities Operations), a multi-investigator facility for the study of combustion science and technology. In-house BES-supported efforts combine theory, modeling, and experiment including diagnostic development, kinetics, and dynamics. Several innovative non-intrusive optical diagnostics such as degenerate four-wave mixing, cavity ring-down spectroscopies, high-resolution optical spectroscopy, and ion-imaging techniques have been developed to characterize gas phase processes. Other activities at the Combustion Research Facility involve BES interactions with the Office of Fossil Energy, the Office of Energy Efficiency and Renewable Energy, and industry.

This activity contributes significantly to DOE missions, since nearly 85 percent of the Nation's energy supply has its origins in combustion and this situation is likely to persist for the foreseeable future. The complexity of combustion -- the interaction of fluid dynamics with hundreds of chemical reactions involving dozens of unstable chemical intermediates -- has provided an impressive challenge to predictive modeling of combustion processes. The chemical physics program supports the development of theories and computational algorithms to predict the rates of chemical reactions at temperatures characteristic of combustion. It supports the development and application of experimental techniques for characterizing gas phase reactions in sufficient detail to develop, test, and validate predictive models of chemical reaction rates. Predicted and measured reaction rates will be

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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used in models for the design of new combustion devices with maximum energy efficiency and minimum, undesired environmental consequences.

The research in chemical dynamics at surfaces is aimed at developing predictive theories for surface mediated chemistry such as is encountered in industrial catalysis or environmental processes. Surface mediated catalysis reduces the energy demands of industrial chemical processes by bypassing energy barriers to chemical reaction. Surface mediated catalysis is used to remove pollutants from combustion emissions. New catalysts are few; improvements come principally from modification of known catalytic materials. There is no body of organized knowledge such as exists for the field of organic chemistry that can be used to find new catalysts for new or existing processes. The knowledge gained from this research program will guide in the development of a predictive capability for surface chemistry.

Capital equipment is provided for such items as picosecond and femtosecond lasers, high-speed detectors, spectrometers and computational resources.

▪ **Photochemistry and Radiation Research** ..... **26,298**    **26,064**    **29,163**

This activity supports fundamental molecular level research on the capture and conversion of energy in the condensed phase. Fundamental research in solar photochemical energy conversion supports organic and inorganic photochemistry, photoinduced electron and energy transfer in the condensed phase, photoelectrochemistry, biophysical aspects of photosynthesis, and biomimetic assemblies for artificial photosynthesis. Fundamental research in radiation chemistry supports chemical effects produced by the absorption of energy from ionizing radiation. The radiation chemistry research encompasses heavy ion radiolysis, models for track structure and radiation damage, characterization of reactive intermediates, radiation yields, and radiation-induced chemistry at interfaces. Accelerator-based electron pulse radiolysis methods are employed in studies of highly reactive transient intermediates, and kinetics and mechanisms of chemical reactions in the liquid phase and at liquid/solid interfaces. This activity supports the Notre Dame Radiation Laboratory, a BES collaborative research center, emphasizing research in radiation chemistry.

Solar photochemical energy conversion is a long-range option for meeting the world's future energy needs. An alternative to semiconductor photovoltaic cells, the attraction of solar photochemical and photoelectrochemical conversion is that fuels, chemicals and electricity may be produced with minimal environmental pollution and with closed renewable energy cycles. Artificial photosynthesis can be coupled to chemical reactions for generation of fuels such as hydrogen, methane, or complex hydrocarbons found in gasoline. The fundamental concepts devised for highly efficient excited-state charge separation in molecule-based biomimetic assemblies should also be applicable in the future development of molecular optoelectronic devices. A strong interface with EE solar conversion programs exists at NREL, involving shared research, analytical and fabrication facilities, and involving a jointly shared project on dye-sensitized solar cells.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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Radiation chemistry research supports fundamental chemical effects produced by the absorption of energy from ionizing radiation. This research is important for solving problems in environmental waste management and remediation, nuclear energy production, and medical diagnosis and radiation therapy. Fundamental studies on radiation-induced processes complement collocated NERI and EMSP projects.

This activity is the dominant supporter (85%) of solar photochemistry in the U.S., and the sole supporter of radiation chemistry.

An increase is requested in FY 2003 for photochemistry and radiation research for studies of nanoscale structures important to photochemical energy conversion. New opportunities offered by nanoscale science, engineering and technology have enabled studies of artificial and biological self-assembled membranes to isolate and optimally configure chromophores to act as electron-donors and acceptors for efficient charge separation that will allow the desired reaction pathways to be controlled. In addition, studies of quantum dots having unique spectral and electrical properties have the potential to revolutionize direct solar to electrical energy conversion. For FY 2003 research will continue to expand our knowledge of the semiconductor/liquid interface, colloidal semiconductors, and dye-sensitized solar cells; inorganic/organic donor-acceptor molecular assemblies and photocatalytic cycles; biophysical studies of photosynthetic antennae and the reaction center; and radiolytic processes at interfaces, radiolytic intermediates in supercritical fluids, and characterization of excited states by dual pulse radiolysis/photolysis experiments.

Capital equipment is provided for such items as pico- and femtosecond lasers, fast Fourier transform-infrared and Raman spectrometers, and upgrades for electron paramagnetic resonance spectroscopy.

▪ **Molecular Mechanisms of Natural Solar Energy Conversion**      **12,345**      **12,150**      **12,150**

This activity, part of the formerly separate Energy Biosciences subprogram, supports fundamental research to characterize the molecular mechanisms involved in the conversion of solar energy to biomass, biofuels, bioproducts, and other renewable energy resources. Research supported includes the characterization of the energy transfer processes occurring during photosynthesis, the kinetic and catalytic mechanisms of enzymes involved in the synthesis of methane, the biochemical mechanisms involved in the synthesis and degradation of lignocellulosics, and the mechanisms of plant oil production. The approaches used include biophysical, biochemical, and molecular genetic analyses. The goal is to enable the future biotechnological exploitation of these processes and, also, to provide insights and strategies into the design of non-biological processes. This activity also encourages fundamental research in the biological sciences that interfaces with other traditional disciplines in the physical sciences.

▪ **Metabolic Regulation of Energy Production**.....      **19,508**      **19,224**      **19,224**

This activity, part of the formerly separate Energy Biosciences subprogram, supports fundamental research in regulation of metabolic pathways and the integration of multiple pathways that constitute cellular function. The potential to synthesize an almost limitless variety of energy-rich organic

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FY 2001	FY 2002	FY 2003
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compounds and polymers exists within the genetic diversity of plants and microbes. Understanding and realizing this potential is founded upon characterizing the genetic makeup of the organism and the regulation of these genes by physical and biological parameters. The research goal is to develop a predictive and experimental context for the manipulation and direction of metabolism to accumulate a desired product. Research supported includes the identification and characterization of genes and gene families within the context of metabolic pathways and their regulation by signaling pathways that can impact energy production; this includes understanding the transduction of signals received from physical sources (e.g. light, temperature, solid surfaces) at the interface between the organism and its environment, as well as the transduction of signals received from biological sources (e.g. developmental programs, symbiotic or syntrophic relationships, nutrient availability).

In FY 2003, studies will continue on *Arabidopsis* as a model system for the study of other plant systems with broader utility. Increased emphasis will be placed upon understanding interactions that occur within the nanoscale range; this includes signal reception at biological surfaces and membranes and catalytic and enzyme-substrate recognition and how these molecules transfer within and between cellular components. This new activity constitutes the fundamental biological advances needed to complement the chemical nanoscale catalysis activities. An emerging area will be the development of new imaging tools and methods to examine metabolic and signaling pathways and to visualize cellular architecture, at both the physical-spatial and temporal scale.

▪ **Catalysis and Chemical Transformation** ..... **25,464**    **24,779**    **31,333**

This activity supports basic research to understand the chemical aspects of catalysis, both heterogeneous and homogeneous; the chemistry of fossil resources; and the chemistry of the molecules used to create advanced materials. While the “art” of catalysis is widely practiced in industry, the fundamental scientific principles that enable predictability are lacking. This activity seeks to develop these principles to enable rational design of catalysts.

Catalytic transformations impact virtually all of the energy missions of the Department. Catalysts are needed for all of the processes required to convert crude petroleum into a clean burning fuel. This is becoming more and more important as petroleum supplies diminish and demands for cleaner burning fuels increase. Also, the production of virtually every chemical-based consumer product requires catalysts at some point. Catalysts are crucial to energy conservation in creating new, less-energy-demanding routes for the production of basic chemical feedstocks and value-added chemicals. Catalysts are also indispensable for processing and manufacturing fuels that are a primary means of energy storage. Environmental impacts from catalytic science can include minimizing unwanted products from production streams and transforming toxic chemicals into benign ones, such as chlorofluorocarbons into environmentally acceptable refrigerants. Research supported by this program also provides the basis and impetus for creating a broad range of new materials, such as mesoporous solids that can act as improved catalysts.

This activity is the Nation’s major supporter of catalysis research, and it is the only activity that treats catalysis as a discipline integrating all aspects of homogeneous and heterogeneous catalysis research.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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Included within this request are funds to increase x-ray and neutron science activities in the U.S. based on BES reviews of the synchrotron radiation light sources, on discussions within the OSTP Interagency Working Group on Neutron Science, and on three BESAC reviews that addressed the current status of research activities using neutron scattering in the U.S. and strategies needed to take full advantage of the SNS upon its completion. Funding is increased for new and upgraded instrumentation to take advantage of scientific opportunities in the physical sciences and to leverage the multibillion-dollar investment in these facilities. Funds will be competed among both laboratory and academic institutions for multiyear beamline and instrument development projects in the range \$5,000,000-15,000,000 each in both homogeneous and heterogeneous catalysis

In FY 2003 research will continue to focus on understanding the unique catalytic properties of metal, as well as mixed metal and oxide particles and their role in catalyzing reactions enabled by nanoscience engineering and technology. Increased emphasis will also be placed on the properties of reactions within nanoscale cavities. Key to these efforts will be studies on the structure, function, and reactivity of metal containing structures both in solution as well as on supports or isolated within three dimensional structures, all within the nanoscale size regime. These activities will focus on understanding the role of nanoscale properties of catalytic materials in controlling chemical reactivity through control of transitions states. Other activities will include the synthesis of discrete nanomaterials created from a controlled assembly of molecular building blocks. Capital equipment is provided for such items as ultrahigh vacuum equipment with various probes of surface structure, Fourier-transform infrared instrumentation, and high-field, solid-state Nuclear Magnetic Resonance (NMR) spectrometers

▪ **Separations and Analyses**..... **14,393**    **12,967**    **14,407**

This activity supports fundamental research covering a broad spectrum of separation concepts, including membrane processes, extraction under both standard and supercritical conditions, adsorption, chromatography, photodissociation, and complexation. Also supported is work to improve the sensitivity, reliability, and productivity of analytical determinations and to develop entirely new approaches to analysis. This activity is the Nation’s most significant long-term investment in many aspects of separations and analysis, including solvent extraction, ion exchange, and mass spectrometry. The goal of this activity is to obtain a thorough understanding of the basic chemical and physical principles involved in separations systems and analytical tools so that their utility can be realized. Work is closely coupled to the Department’s stewardship responsibility for transuranic chemistry and for the Environmental Management clean-up mission; therefore, separation and analysis of transuranic isotopes and their radioactive decay products are important components of the portfolio.

Knowledge of molecular level processes is required to characterize and treat extremely complex radioactive mixtures and to understand and predict the fate of associated contaminants in the environment. Though the cold war legacy is the most obvious of the Department’s missions, the economic importance of separation science and technology is huge. For example, distillation

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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processes in the petroleum, chemical, and natural gas industries annually consume the equivalent of 315 million barrels of oil. It has been estimated that separation processes account for more than 5 percent of total national energy consumption. Separations are essential to nearly all operations in the processing industries and are also necessary for many analytical procedures. An analysis is an essential component of every chemical process from manufacture through safety and risk assessment and environmental protection.

Studies in at the nanoscale address molecular transport in nanoscale structures as well as the formation of macroscopic separation systems via self-assembly of nanoscale precursors. Increased funding in FY 2003 is requested for separations and analysis research to address fundamental questions of how individual molecules move on membrane surfaces and within the pores resulting in molecular separations and transformations. This work will build on recent advances in imaging single-molecule interactions and reactions and will expand our knowledge of how molecules interact with pore walls, with one another, and with other molecules to effect separation between molecules.

Capital equipment is provided for such items as computational workstations and inductively coupled plasma torch spectrometers for atomic emission determination.

▪ **Heavy Element Chemistry** ..... **8,154**      **7,637**      **8,637**

This activity supports research in actinide and fission product chemistry. Areas of interest include aqueous and non-aqueous coordination chemistry; solution and solid-state speciation and reactivity; measurement of chemical and physical properties; synthesis of actinide-containing materials; chemical properties of the heaviest actinide and transactinide elements; theoretical methods for the prediction of heavy element electronic and molecular structure and reactivity; and the relationship between the actinides, lanthanides, and transition metals.

The heavy element chemistry program, with its genesis in the Manhattan project, has explored the chemical properties of the transuranium and transactinide elements, the latter using techniques developed for isotopes that have half-lives on the order of seconds to tens of seconds. In recent years the emphasis of the program returned to the chemistry of the lighter transuranium elements and fission products, driven by the necessity to identify species found in the waste tanks at the Hanford and Savannah River sites. Knowledge of the molecular speciation of actinide and fission products materials under tank conditions is necessary to treat these complex mixtures. Accidental release of actinide and fission product materials to the environment also requires molecular speciation information in order to predict their fate under environmental conditions. This activity is closely coupled to the BES separations and analysis activity and to the actinide and fission product chemistry efforts in DOE's Environmental Management Science Program.

This activity represents the Nation's only funding for basic research in the chemical and physical principles of actinide and fission product materials. The program is primarily based at the national laboratories because of the special licenses and facilities needed to obtain and safely handle radioactive materials. However, research in heavy element chemistry is supported at universities, and collaborations between university and laboratory programs are encouraged. The training of graduate

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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students and postdoctoral research associates is viewed as an important responsibility of this activity.

Approximately twenty undergraduate students chosen from universities and colleges throughout the U.S. are given introductory lectures in actinide and radiochemistry each summer.

Increased funding in FY 2003 is requested for research in the chemistry of transuranic elements, particularly the role of f-orbital electrons in the coordination chemistry of neptunium, plutonium, americium, and curium. The involvement of the f-orbital electrons in chemical bonding occurs most frequently in the actinide elements and particularly those elements most uniquely associated with the Department of Energy's defense and environmental missions. Experiment combined with theory and modeling will lead to new understanding of chemical bonding in these elements. Experimental studies will include aqueous and non-aqueous high-pressure chemistry and surface chemistry of these elements. In addition, new beamlines at synchrotron light sources capable of handling samples of these heavy elements will permit detailed spectroscopic studies of specimens under a variety of conditions. The study of the bonding in these heavy elements may also provide new insights into organometallic chemistry, beyond that learned from "standard" organometallic chemistry based on transition metals with d-orbital bonding.

Capital equipment is provided for items used to characterize actinide materials (spectrometers, ion chambers, calorimeters, etc.) and equipment for synchrotron light source experiments to safely handle the actinides.

▪ **Geosciences Research** ..... **21,419**      **21,262**      **21,262**

The Geosciences activity supports long term basic research in geochemistry and geophysics. Geochemical research focuses on subsurface solution chemistry, mineral-fluid interactions, and isotopic distributions and migration in natural systems. Geophysical research focuses on new approaches to understand physical properties of fluids, rocks and minerals. It seeks fundamental understanding of the physics of wave propagation in complex media ranging from single crystals to the scale of the earth's crust. This activity has pioneered the application of x-ray and neutron scattering to geochemical and geophysical studies.

These studies provide the fundamental science base for new capabilities to locate and monitor oil and gas reservoirs, contaminant migration, and for characterizing disposal sites for energy related wastes. Research also seeks to understand the fundamental geological processes that impact concepts for sequestration of carbon dioxide in subsurface reservoirs. This activity provides the majority of individual investigator basic research funding for the federal government in areas with the greatest impact on unique DOE missions such as high-resolution Earth imaging and low-temperature, low-pressure geochemical processes in the subsurface. This activity provides the basic research component in solid Earth sciences to the DOE's energy resources and environmental quality portfolios.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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▪ **Chemical Energy and Chemical Engineering** ..... **12,679**    **10,953**    **10,953**

This activity supports research on electrochemistry, thermophysical and thermochemical properties, and physical and chemical rate processes. Also included is fundamental research in areas critical to understanding the underlying limitations in the performance of electrochemical energy storage and conversion systems including anode, cathode, and electrolyte systems and their interactions with emphasis on improvements in performance and lifetime. The program covers a broad spectrum of research including fundamental studies of composite electrode structures; failure and degradation of active electrode materials; thin film electrodes, electrolytes, and interfaces; and experimental and theoretical aspects of phase equilibria, especially of mixtures, including supercritical phenomena.

Knowledge of bulk behavior of chemicals and mixtures based on molecular properties is required for the design of energy efficient chemical processes in all aspects of plant design across the entire spectrum of industrial activities. The thermophysical and thermochemical properties of molecules provide the basis for developing equations of states and parameters for fluid models that are necessary for the development of engineering designs that maximize the efficiency of all energy production, storage, and consumption devices. These engineering designs are also an essential component of safety and risk assessment and environmental protection.

In the area of energy storage coordination of fundamental and applied research efforts across the government is accomplished by participation in the Interagency Power Working Group. Close coordination with the Battery and Fuel Cell programs in EE-Office of Transportation Technologies is accomplished through joint program meetings, workshops, and strategy sessions.

For FY 2003, there will be continued emphasis on research to expand the ability to control electrode structures on the nanometer scale. Preliminary studies have shown that this has a great impact on the electrochemical efficiency of electrode processes and the rate at which they respond to electrochemical potentials.

Capital equipment is provided for such items as computer work stations and electrochemical apparatus.

▪ **General Plant Projects (GPP)** ..... **11,524**    **12,170**    **12,210**

GPP funding is for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems principally at the Ames Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory as part of the Basic Energy Sciences stewardship responsibilities for these laboratories. Funding of this type is essential for maintaining the productivity and usefulness of the Department-owned facilities and in meeting requirements for safe and reliable facilities operation. Additional GPP funding is included in the Facilities Operations justification in both the Materials Sciences and Engineering subprogram and the Chemical Sciences, Geosciences, and Energy Biosciences subprogram. The total estimated cost of each GPP project will not exceed \$5,000,000.



(dollars in thousands)

FY 2001	FY 2002	FY 2003
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▪ **General Purpose Equipment (GPE)**..... **4,081**      **3,655**      **4,180**

GPE funding is provided for Ames Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory as part of the Basic Energy Sciences stewardship responsibilities for these laboratories for general purpose equipment that supports multipurpose research. Increased infrastructure funding is requested to maintain, modernize, and upgrade ORNL, ANL, and Ames site and facilities to correct deficiencies due to aging, changing technology, and inadequate past investments.

▪ **SPEAR3 Upgrade** ..... **1,700**      **700**      **700**

Over the period FY 1999 - FY 2003, the SPEAR3 upgrade (funded in both BES subprograms) is being undertaken at SSRL to provide major improvements to all existing experimental stations served by this synchrotron radiation light source. The technical goals are to increase injection energy from 2.3 GeV to 3 GeV to improve the energy spectrum available to users; decrease beam emittance by a factor of 7 to increase beam brightness; increase operating current from 100 mA to 200 mA to increase beam intensity; and maintain long beam life time (>25 hr). The increased photon flux will greatly improve performance in a variety of applications including powder and thin film diffraction, topographic studies, surface microcontamination studies, x-ray tomographic analysis, x-ray absorption studies, and protein crystallography. The magnets and associated vacuum chambers of the existing SPEAR storage ring will be replaced in order to implement the revised lattice system. All components are housed within the existing buildings. The TEC is \$29,000,000; DOE and NIH are equally funding the upgrade with a total Federal cost of \$58,000,000. NIH has provided \$14,000,000 in FY 1999, \$14,000,000 in FY 2000, and \$1,000,000 in FY 2001. The funding profile, but not the TEC, of this MIE has been modified based on an Office of Science construction project review, which recommended that some funds be shifted from later years to early years in order to reduce schedule risk by ensuring that critical components are available for installation when scheduled. That recommendation was accepted and is reflected in the current funding profile. **Performance will be measured** by continuing upgrades on the major components of the SPEAR3, maintaining cost and schedule within 10% of baselines. The increased brightness for all experimental stations at SSRL will greatly improve performance in a variety of applications and scientific studies. This subprogram funds the Combustion Research Facility. The x-ray and neutron scattering facility operations, formerly funded in Chemical Sciences, are now funded in the Materials Sciences and Engineering subprogram.

▪ **Advanced Light Source Beamline** ..... **900**      **975**      **0**

This beamline is a major item of equipment with a total estimated cost of \$6,000,000 that will provide capabilities for surface and interfacial science important to geosciences, environmental science, and aqueous corrosion science. It is being funded jointly by the Materials Sciences and Engineering subprogram and the Chemical Sciences, Geosciences, and Energy Biosciences subprogram.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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**Facility Operations**..... **5,463**      **5,377**      **5,805**

The facility operations budget request, which includes operating funds, capital equipment, and general plant projects is described in a consolidated manner later in this budget. This subprogram funds the Combustion Research Facility. General Plant Project (GPP) funding is also required for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems. The total estimated cost of each GPP project will not exceed \$5,000,000. The x-ray and neutron scattering facility operations, formerly funded in Chemical Sciences, are now funded in the Materials Sciences and Engineering subprogram.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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Facilities

Combustion Research Facility..... 5,463      5,377      5,805

Total, Facilities..... 5,463      5,377      5,805

(dollars in thousands)

FY 2000	FY 2001	FY 2002
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**SBIR/STTR**..... **0**      **4,770**      **5,022**

In FY 2001, \$4,646,000 and \$279,000 were transferred to the SBIR and STTR programs, respectively. The FY 2002 and FY 2003 amounts shown are the estimated requirement for the continuation of the SBIR and STTR programs.

**Total, Chemical Sciences, Geosciences, and Energy Biosciences**      **203,231**      **207,783**      **220,146**

### Explanation of Funding Changes from FY 2002 to FY 2003

FY 2003 vs. FY 2002 (\$000)
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#### Chemical Sciences, Geosciences, and Energy Biosciences Research

- Increase in photochemistry and radiation research for studies of nanoscale structures important to photochemical energy conversion..... +3,099
- Increase in catalysis research to understand the role nanoscale properties play in altering and controlling catalytic transformations. .... +6,554

FY 2003 vs. FY 2002 (\$000)
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▪ Increase for chemical separations and analysis research on how individual molecules move on membrane surfaces and within the pores resulting in molecular separations and transformations. ....	+1,440
▪ Increase in heavy element chemistry research in the chemistry of transuranic elements, particularly the role of f-orbital electrons in the coordination chemistry of neptunium, plutonium, americium, and curium.....	+1,000
▪ Increase in General Plant Projects .....	+40
▪ Increase in General Purpose Equipment.....	+525
▪ Decrease in capital equipment funding for the ALS Beamline MIE per approved funding profile .....	-975
Total, Chemical Sciences, Geosciences, and Energy Biosciences Research .....	+11,683
<b>Facilities Operations</b>	
▪ Increase for operations of the Combustion Research Facility. ....	+428
Total, Chemical Sciences, Geosciences, and Energy Biosciences Facilities Operations.	+428
<b>SBIR/STTR</b>	
▪ Increase SBIR/STTR funding because of increase in operating expenses. ....	+252
Total Funding Change, Chemical Sciences, Geosciences, and Energy Biosciences .....	+12,363

# Construction

## Mission Supporting Goals and Objectives

Construction is needed to support the research in each of the subprograms in the Basic Energy Sciences program. Experiments necessary in support of basic research require that state-of-the-art facilities be built or existing facilities modified to meet unique research requirements. Reactors, radiation sources, and neutron sources are among the expensive, but necessary, facilities required. The budget for the BES program includes funding for the construction and modification of these facilities.

### Funding Schedule

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
SNS .....	258,929	276,300	210,571	-65,729	-23.8%
Project Engineering Design, NSRCs .....	0	3,000	11,000	+8,000	+266.7%
Project Engineering Design, LCLS .....	0	0	6,000	+6,000	--
Center for Nanophase Materials Science (ORNL) .....	0	0	24,000	+24,000	--
<b>Total, Construction .....</b>	<b>258,929</b>	<b>279,300</b>	<b>251,571</b>	<b>-27,729</b>	<b>-9.9%</b>

### Detailed Program Justification

(dollars in thousands)

	FY 2001	FY 2002	FY 2003
<b>Construction .....</b>	<b>258,929</b>	<b>279,300</b>	<b>251,571</b>
<b>Spallation Neutron Source .....</b>	<b>258,929</b>	<b>276,300</b>	<b>210,571</b>

FY 2003 funding is requested to continue instrument R&D and design, procurement, construction, and installation activities, and to begin system commissioning. The front end will be commissioned, and low-energy linac component installation and commissioning will commence. Other linac and ring components will begin to be delivered and installed in their respective tunnels. Target building construction and equipment installation will continue in concert with each other. Numerous conventional facilities including the klystron, central utilities, and ring service buildings as well as the linac and ring tunnels will be completed. All site utilities will be available to support linac commissioning activities. **Performance will be measured** by continued construction of the SNS, meeting the cost and timetables within 10% of the baseline in the construction project data sheet. Once completed in mid-2006, the SNS will provide beams of neutrons used to probe and understand the physical, chemical, and biological properties of materials at an atomic level, leading to improvements in high technology industries. Additional information follows later in construction project data sheet 99-E-334.

(dollars in thousands)

FY 2001	FY 2002	FY 2003
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**Project Engineering and Design, Nanoscale Science Research Centers**..... **0 3,000 11,000**

FY 2003 budget authority is requested to provide Title I and Title II design-only funding for Nanoscale Science Research Centers (NSRCs) at Oak Ridge National Laboratory, Lawrence Berkeley National Laboratory, and Sandia National Laboratory to assure project feasibility, define the scope, and provide estimates of construction costs and schedules. NSRCs will provide state-of-the-art facilities for materials nanofabrication and advanced tools for nanocharacterization to the scientific community. Additional information follows later in PED data sheet 02-SC-002.

**Project Engineering and Design, Linac Coherent Light Source.** **0 0 6,000**

FY 2003 budget authority is requested to provide Title I and Title II design-only funding for the Linac Coherent Light Source (LCLS) at SLAC to assure project feasibility, define the scope, and provide estimates of construction costs and schedules. The LCLS will provide laser-like radiation in the x-ray region of the spectrum that is 10 orders of magnitude (i.e., a factor of 10,000,000,000) greater in peak power and peak brightness than any existing coherent x-ray light source. Additional information follows later in PED data sheet 03-SC-002.

**Nanoscale Science Research Center – The Center for Nanophase Materials Sciences, ORNL**..... **0 0 24,000**

FY 2003 funding is requested for the start of construction of the Center for Nanophase Materials Science to be located at Oak Ridge National Laboratory. **Performance will be measured** by meeting the cost and timetables within 10% of the baseline in the construction project data sheet. Additional information follows later in construction project data sheet 03-R-312.

**Total, Construction**..... **258,929 279,300 251,571**

## Explanation of Funding Changes from FY 2002 to FY 2003

FY 2003 vs. FY 2002 (\$000)
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### Construction

<ul style="list-style-type: none"> <li>▪ The decrease in funding for the Spallation Neutron Source represents the scheduled ramp down of activities. ....</li> <li>▪ Increase in Project Engineering and Design for Nanoscale Science Research Centers at ORNL, LBNL, and SNL.....</li> <li>▪ Increase in funding for the start of construction of the Center for Nanophase Materials Science to be located at ORNL.....</li> <li>▪ Increase in funding for Project Engineering Design related to design-only activities for the Linac Coherent Light Source (LCLS).....</li> </ul>	-65,729  +8,000  +24,000  +6,000
Total Funding Change, Construction .....	-27,729

# Major User Facilities

## Mission Supporting Goals and Objectives

The BES scientific user facilities provide experimental capabilities that are beyond the scope of those found in laboratories of individual investigators. Synchrotron radiation light sources, high-flux neutron sources, electron beam microcharacterization centers, and other specialized facilities enable scientists to carry out experiments that could not be done elsewhere. These facilities are part of the Department's system of scientific user facilities, the largest of its kind in the world. A description of each facility is provided in the "Site Descriptions" section. Any unusual or nonrecurring aspects of funding are described in the following section "Detailed Program Justification."

The facilities are planned in collaboration with the scientific community and are constructed and operated by BES for support of forefront research in areas important to BES activities and also in areas that extend beyond the scope of BES activities such as structural biology, medical imaging, and micro machining. These facilities are used by researchers in materials sciences, chemical sciences, earth and geosciences, environmental sciences, structural biology, superconductor technology, and medical research and technology development. The facilities are open to all qualified scientists from academia, industry, and the federal laboratory system whose intention is to publish in the open literature. The funding schedule includes only those facilities that have operating budgets for personnel, utilities, and maintenance.

## Funding Schedule

Funding for the operation of these facilities is provided in the Materials Sciences and Engineering and the Chemical Sciences, Geosciences, and Energy Biosciences subprograms.

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
Advanced Light Source.....	35,605	37,009	39,561	+2,552	+6.9%
Advanced Photon Source.....	90,314	87,380	91,291	+3,911	+4.5%
National Synchrotron Light Source.....	34,720	33,671	35,893	+2,222	+6.6%
Stanford Synchrotron Radiation Laboratory.....	21,696	21,357	22,673	+1,316	+6.2%
High Flux Beam Reactor.....	15,341	0	0	0	--
High Flux Isotope Reactor .....	37,197	37,872	36,854	-1,018	-2.7%
Radiochemical Engineering Development Center ..	6,512	6,606	6,712	+106	+1.6%
Intense Pulsed Neutron Source.....	13,833	15,826	17,015	+1,189	+7.5%
Manuel Lujan, Jr. Neutron Scattering Center.....	9,190	9,044	9,678	+634	+7.0%
Spallation Neutron Source .....	19,059	15,100	14,441	-659	-4.4%
Combustion Research Facility.....	5,463	5,377	5,805	+428	+8.0%
<b>Total, Major User Facilities.....</b>	<b>288,930</b>	<b>269,242</b>	<b>279,923</b>	<b>+10,681</b>	<b>+4.0%</b>

## Detailed Program Justification

(dollars in thousands)

	FY 2001	FY 2002	FY 2003
<b>Major User Facilities</b> .....	<b>288,930</b>	<b>269,242</b>	<b>279,923</b>
▪ Advanced Light Source at Lawrence Berkeley National Laboratory.....	35,605	37,009	39,561
▪ Advanced Photon Source at Argonne National Laboratory.....	90,314	87,380	91,291
▪ National Synchrotron Light Source at Brookhaven National Laboratory.....	34,720	33,671	35,893
▪ Stanford Synchrotron Radiation Laboratory at Stanford Linear Accelerator Center.....	21,696	21,357	22,673
▪ High Flux Beam Reactor at Brookhaven National Laboratory. On November 16, 1999, Secretary Richardson announced the permanent closure of the reactor. Responsibility has been transferred from SC to the Office of Environmental Management for surveillance and decommissioning.....	15,341	0	0
▪ High Flux Isotope Reactor at Oak Ridge National Laboratory. ...	37,197	37,872	36,854
▪ Radiochemical Engineering Development Center (REDC) at Oak Ridge National Laboratory. ....	6,512	6,606	6,712
▪ Intense Pulsed Neutron Source at Argonne National Laboratory.	13,833	15,826	17,015
▪ Manuel Lujan, Jr. Neutron Scattering Center at Los Alamos National Laboratory.....	9,190	9,044	9,678
▪ Spallation Neutron Source at Oak Ridge National Laboratory. ...	19,059	15,100	14,441
▪ Combustion Research Facility at Sandia National Laboratories/California.....	5,463	5,377	5,805
<b>Total, Major User Facilities</b> .....	<b>288,930</b>	<b>269,242</b>	<b>279,923</b>



# Capital Operating Expenses & Construction Summary

## Capital Operating Expenses

(dollars in thousands)

	FY 2001	FY 2002	FY 2003	\$ Change	% Change
General Plant Projects.....	11,874	12,518	12,570	+52	+0.4%
Accelerator Improvement Projects.....	11,935	11,577	9,067	-2,510	-21.7%
Capital Equipment .....	62,165	62,235	76,249	+14,014	+22.5%
<b>Total, Capital Operating Expenses.....</b>	<b>85,974</b>	<b>86,330</b>	<b>97,886</b>	<b>+11,556</b>	<b>+13.4%</b>

## Construction Projects

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Appropriations	FY 2001	FY 2002	FY 2003	Unappropriated Balances
99-E-334 Spallation Neutron Source, ORNL .....	1,192,700	201,400	258,929	276,300	210,571	245,500
02-SC-002 PED, Nanoscale Science Research Centers.....	15,000 <sup>a</sup>	0	0	3,000	11,000	1,000
03-SC-002, PED, Stanford Linear Accelerator Center.....	33,500 <sup>b</sup>	0	0	0	6,000	27,500
03-R-312, ORNL, Center for Nanophase Material Sciences .....	64,250	0	0	0	24,000	40,250
<b>Total, Construction.....</b>		<b>201,400</b>	<b>258,929</b>	<b>279,300</b>	<b>251,571</b>	<b>314,250</b>

<sup>a</sup> The full Total Estimated Cost (design and construction) ranges between \$160,000,000 and \$235,000,000. This estimate is based on conceptual data and should not be construed as a project baseline.

<sup>b</sup> The full TEC Projection (design and construction) ranges between \$165,000,000 and \$225,000,000. This is a preliminary estimate based on conceptual data and should not be construed as a project baseline.

## Major Items of Equipment (TEC \$2 million or greater)

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Approp- riations	FY 2001	FY 2002	FY 2003 Request	Accept- ance Date
HB-2 Beam Tube Extension at HFIR - ORNL.....	5,550	4,400	1,150	0	0	FY 2001
SPEAR3 Upgrade.....	29,000 <sup>a</sup>	0	10,000	9,000	10,000	FY 2003
ALS Beamline.....	6,000	2,250	1,800	1,950	0	FY 2003
Total, Major Items of Equipment .....		6,650	12,950	10,950	10,000	

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<sup>a</sup> DOE portion only; total estimated Federal cost, including NIH funding (beginning in FY 1999), is \$58,000,000.

# 99-E-334 – Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee

(Changes from FY 2002 Congressional Budget Request are denoted with a vertical line in the left margin.)

## Significant Changes

Clarifying language has been added to Sections 2 and 3 with respect to scientific instruments that are related to, but not a part of, the SNS Project.

Estimate of related Annual Funding Requirements has been updated in Section 7.

### 1. Construction Schedule History

	Fiscal Quarter				Total Estimated Cost (\$000)	Total Project Cost (\$000)
	A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
FY 1999 Budget Request (Preliminary Estimate) .....	1Q 1999	4Q 2003	3Q 2000	4Q 2005	1,138,800	1,332,800
FY 2000 Budget Request .....	1Q 1999	4Q 2003	3Q 2000	1Q 2006	1,159,500	1,360,000
FY 2001 Budget Request .....	1Q 1999	4Q 2003	3Q 2000	3Q 2006	1,220,000	1,440,000
FY 2001 Budget Request ( <i>Amended</i> ) ..	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,192,700	1,411,700
FY 2002 Budget Request.....	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,192,700	1,411,700
FY 2003 Budget Request ( <i>Current Estimate</i> ).....	1Q 1999	4Q 2003	1Q 2000	3Q 2006	1,192,700	1,411,700

## 2. Financial Schedule <sup>1</sup>

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
1999	101,400	101,400	37,140
2000	100,000	100,000	105,542
2001	258,929	258,929	170,453
2002	276,300	276,300	287,732
2003	210,571	210,571	301,304
2004	124,600	124,600	159,752
2005	79,800	79,800	83,146
2006	41,100	41,100	47,631

<sup>1</sup> In FY 2001, two grants were awarded to universities for research covering the design, fabrication and installation of instruments for neutron scattering. Both awards were made based on competitive peer review under 10CFR Part 605, Financial Assistance Program. Both instruments will be located at the SNS. These awards follow the advice of the Basic Energy Sciences Advisory Committee, that the Department should "expand the university base for neutron scattering. The only way to build the user base required to be internationally competitive is to enhance the participation from academic institutions. An immediate injection of funds to support the exploitation of pulsed neutron sources for science by the U.S. academic community is needed." Several universities participate in these grants, including MIT, University of California, University of Delaware, University of Colorado, University of Utah, Johns Hopkins, University of New Mexico, and Syracuse University. Pennsylvania State University submitted an application on April 12, 2001. After peer review the award to Pennsylvania State University was made for 5 years, starting August 15, 2001, and ending August 14, 2006, for a total of \$12,824,168 of operating funds for an instrument for research in inelastic neutron scattering, quantum liquids, magnetism, environmental chemistry, polymer dynamics, and lubrication. This instrument will be owned by Pennsylvania State University.

The California Institute of Technology submitted an application on June 11, 2001. After peer review, the award to California Institute of Technology was made for 5 years, starting September 15, 2001, and ending September 14, 2006, for a total of \$11,579,000 of operating funds for an instrument for research in lattice dynamics, magnetic dynamics, chemical physics, and characterization of novel materials. This instrument will be owned by California Institute of Technology.

In addition to the two above identified instruments, the Basic Energy Sciences program will provide \$5,000,000 of Materials Sciences and Engineering subprogram funding in FY 2003 to continue the development of instrumentation to exploit the scientific potential of the SNS facility. These instruments will be built by individual DOE laboratories or consortia of DOE laboratories in collaboration with the SNS based on scientific merit and importance to users from universities, industries, and government laboratories. The instruments will be operated for users by the SNS based on applications for experiments selected competitively by the peer review procedures established for access to the SNS. See further discussion in Materials Sciences and Engineering subprogram under X-ray and Neutron Scattering.

### 3. Project Description, Justification and Scope <sup>1</sup>

The purpose of the Spallation Neutron Source (SNS) Project is to provide a next-generation short-pulse spallation neutron source for neutron scattering and related research in broad areas of the physical, chemical, materials, biological, and medical sciences. The SNS will be a national facility with an open user policy attractive to scientists from universities, industries, and federal laboratories. It is anticipated that the facility, when in full operation, will be used by 1,000-2,000 scientists and engineers each year and that it will meet the national need for neutron science capabilities well into the 21<sup>st</sup> Century. Neutrons enable scientists studying the physical, chemical, and biological properties of materials to determine how atoms and molecules are arranged and how they move. This is the microscopic basis for understanding and developing materials of technological significance to support information technology, transportation, pharmaceuticals, magnetic, and many other economically important areas.

The importance of neutron science for fundamental discoveries and technological development is universally acknowledged. The scientific justification and need for a new neutron source and instrumentation in the U.S. have been thoroughly established by numerous studies by the scientific community since the 1970s. These include the 1984 National Research Council study *Major Facilities for Materials Research and Related Disciplines* (the Seitz-Eastman Report), which recommended the immediate start of the design of both a steady-state source and an accelerator-based pulsed spallation source. More recently, the 1993 DOE Basic Energy Sciences Advisory Committee (BESAC) report *Neutron Sources for America's Future* (the Kohn Panel Report) again included construction of a new pulsed spallation source with SNS capabilities among its highest priorities. This conclusion was even more strongly reaffirmed by the 1996 BESAC Report (the Russell Panel Report), which recommended the construction of a 1 megawatt (MW) spallation source that could be upgraded to significantly higher powers in the future.

Neutrons are a unique and increasingly indispensable scientific tool. Over the past decade, they have made invaluable contributions to the understanding and development of many classes of new materials, from high temperature superconductors to fullerenes, a new form of carbon. In addition to creating the new scientific knowledge upon which unforeseen breakthroughs will be based, neutron science is at the core of many technologies that currently improve the health of our citizenry and the safety and effectiveness of our industrial materials.

The information that neutrons provide has wide impacts. For example, chemical companies use neutrons to make better fibers, plastics, and catalysts; drug companies use neutrons to design drugs with higher potency and fewer side effects; and automobile manufacturers use the penetrating power of neutrons to understand how to cast and forge gears and brake discs in order to make cars run better and more safely. Furthermore, research on magnetism using neutrons has led to higher strength magnets for more efficient electric generators and motors and to better magnetic materials for magnetic recording tapes and computer hard drives.

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<sup>1</sup> As part of the development of Oak Ridge National Laboratory, other buildings may be located on Chestnut Ridge, which is the site of the SNS and is located just across Bethel Valley Road from improvements planned for the main ORNL campus. For example, the Center for Nanophase Materials Sciences (CNMS) will be located on Chestnut Ridge, because research activities at the CNMS will integrate nanoscale science research with neutron science; synthesis; and theory, modeling, and simulation. The CNMS will be adjacent to the SNS Laboratory – Office Building and will be connected to it by a walkway. See construction project datasheet 03-R-312 for further information on the CNMS.

Based on the recommendations of the scientific community obtained via the Russell Panel Report, the SNS is required to operate at an average power on target of at least 1 megawatt (MW); although the designers had aimed for 2 MW, current projections fall between 1 to 2 MW. At this power level, the SNS will be the most powerful spallation source in the world—many times that of ISIS at the Rutherford Laboratory in the United Kingdom. Furthermore, the SNS is specifically designed to take advantage of improvements in technology, new technologies, and additional hardware to permit upgrades to substantially higher power as they become available. Thus, the SNS will be the nation's premiere neutron facility for many decades.

The importance of high power, and consequently high neutron flux (i.e., high neutron intensity), cannot be overstated. The properties of neutrons that make them an ideal probe of matter also require that they be generated with high flux. (Neutrons are particles with the mass of the proton, with a magnetic moment, and with no electrical charge.) Neutrons interact with nuclei and magnetic fields; both interactions are extremely weak, but they are known with great accuracy. Because they have spin, neutrons have a magnetic moment and can be used to study magnetic structure and magnetic properties of materials. Because they weakly interact with materials, neutrons are highly penetrating and can be used to study bulk phase samples, highly complex samples, and samples confined in thick-walled metal containers. Because their interactions are weak and known with great accuracy, neutron scattering is far more easily interpreted than either photon scattering or electron scattering. However, the relatively low flux of existing neutron sources and the small fraction of neutrons that get scattered by most materials mean that most measurements are limited by the source intensity.

The pursuit of high-flux neutron sources is more than just a desire to perform experiments faster, although that, of course, is an obvious benefit. High flux enables broad classes of experiments that cannot be done with low-flux sources. For example, high flux enables studies of small samples, complex molecules and structures, time-dependent phenomena, and very weak interactions. Put most simply, high flux enables studies of complex materials in real time and in all disciplines—physics, chemistry, materials science, geosciences, and biological and medical sciences. Oak Ridge National Laboratory has extensive research efforts in all of these areas.

The SNS will consist of a linac-ring accelerator system that delivers short (microsecond) pulses to a target/moderator system where neutrons are produced by a nuclear reaction process called spallation. The process of neutron production in the SNS consists of the following: negatively charged hydrogen ions are produced in an ion source and are accelerated to approximately 1 billion electron volts (GeV) energy in a linear accelerator (linac); the hydrogen ion beam is injected into an accumulator ring through a stripper foil, which strips the electrons off of the hydrogen ions to produce a proton beam; the proton beam is collected and bunched into short pulses in the accumulator ring; and, finally, the proton beam is injected into a heavy metal target at a frequency of up to 60 Hz. The intense proton bursts striking the target produce pulsed neutron beams by the spallation process. The high-energy neutrons so produced are moderated (i.e., slowed down) to reduce their energies, typically by using thermal or cold moderators. The moderated neutron beams are then used for neutron scattering experiments. Specially designed scientific instruments use these pulsed neutron beams for a wide variety of investigations.

The primary objectives in the design of the site and buildings for the SNS are to provide optimal facilities for the DOE and the scientific community for neutron scattering well into the 21<sup>st</sup> Century and to address the mix of needs associated with the user community, the operations staff, security, and safety.

A research and development (R&D) program is required to ensure technical feasibility and to determine physics design of accelerator and target systems that will meet performance requirements.

The objectives stated above will be met by the technical components described earlier (ion source; linac; accumulator ring; target station with moderators; beam transport systems; and initial experimental equipment necessary to place the SNS in operation) and attendant conventional facilities. As the project design and construction progresses, value engineering analyses and R&D define changes that are applied to the technical baseline to maximize the initial scientific capability of the SNS within the currently established cost and schedule. Thus the SNS project will be considered complete when all capital facilities necessary to achieve the initial baseline goals have been installed and certified to operate safely and properly. In addition, to the extent possible within the total project cost, provisions will be made to facilitate a progression of future improvements and upgrades aimed at keeping SNS at the forefront of neutron scattering science throughout its operating lifetime. Indeed, the current design contains a number of enhancements (e.g. superconducting radiofrequency acceleration, best-in-class instruments, more instrument stations, and higher energy ring) that provide higher performance than the conceptual design that was the basis of initial project approval.

The scientific user community has advised the DOE Office of Basic Energy Sciences that the SNS should keep pace with developments in scientific instruments. Since the average cost for a state-of-the-art instrument has roughly doubled in recent years, SNS has reduced the number of instruments provided within the project TEC. Although this translates into an initial suite of five rather than the ten instruments originally envisioned, the cumulative scientific capability of the SNS has actually increased more than ten-fold. In order to optimize the overall project installation sequence and early experimental operations, three of these instruments will be installed as part of the project; the other two will be completed, with installation occurring during initial low power operations. As with all scientific user facilities such as SNS, additional and even more capable instruments will be installed over the course of its operating lifetime. Many of these future instruments will be provided by other entities, such as the National Science Foundation, other countries, as well as other DOE programs.

The SNS project made significant progress in FY 2001 towards scheduled milestones. R&D supporting technical component design is now over 90% complete. Project-wide, design work is about 70% complete, with conventional facility Title II design nearly 100% complete. Site preparation was completed, and construction began on the front end and target buildings, the linac tunnel, as well as a number of support buildings and utility systems. A number of procurements for materials and technical components were awarded, with generally favorable cost results, and delivery of some items to Oak Ridge began. Definitive plans for equipment delivery and installation and for handoff of technical systems to Oak Ridge for commissioning activities were developed.

FY 2002 budget authority will be used to continue R&D, design, procurement, and construction activities, and to begin component installation. Essentially all R&D supporting construction of the SNS will be completed, with instrument R&D continuing. Title II design will be completed on the linac, and will continue on the ring, target, and instrument systems. The completed front end ion source and portions of the drift tube linac will be delivered to the site to begin their installation. Other system components for the accelerator, ring, target, and instruments will continue to be manufactured. Work on conventional facilities will continue, with some reaching completion and being turned over for equipment installation, such as the front end building, and portions of the klystron building and linac tunnel. Construction work will begin on the ring tunnel.

FY 2003 budget authority is requested to continue instrument R&D and design, procurement, construction, and installation activities, and to begin system commissioning. The front end will be commissioned, and the drift tube linac will be installed and commissioning begun. Installation of other linac components will proceed and installation of ring components will begin. Target building construction and equipment installation will continue in concert with each other. Numerous conventional facilities, including the klystron, central utilities, and ring service buildings as well as the linac and ring tunnels, will be completed. All site utilities will be available to support linac commissioning activities.

#### 4. Details of Cost Estimate

(dollars in thousands)

	Current Estimate	Previous Estimate
Design and Management Costs		
Engineering, design and inspection at approximately 22% of construction costs .....	159,500	179,400
Construction management at approximately 2% of construction costs .....	14,000	20,400
Project management at approximately 14% of construction costs .....	104,700	121,800
Land and land rights .....	0	0
Construction Costs		
Improvements to land (grading, paving, landscaping, and sidewalks) .....	31,500	28,300
Buildings .....	181,600	173,600
Utilities (electrical, water, steam, and sewer lines) .....	20,900	25,100
Technical Components .....	505,500	441,400
Standard Equipment .....	17,500	1,900
Major computer items .....	5,500	5,300
Design and project liaison, testing, checkout and acceptance .....	31,000	16,600
Subtotal .....	1,071,700	1,013,800
Contingencies at approximately 11% of above costs <sup>1</sup> .....	121,000	178,900
Total Line Item Cost .....	1,192,700	1,192,700
Less: Non-Agency Contribution .....	0	0
Total, Line Item Costs (TEC) .....	1,192,700	1,192,700

<sup>1</sup> The contingency, expressed as a percentage of the remaining effort to complete the line item project, is approximately 20%.



## **5. Method of Performance**

The SNS project is being carried out by a partnership of six DOE national laboratories, led by Oak Ridge National Laboratory, as the prime contractor to DOE. The other five laboratories are Argonne, Brookhaven, Lawrence Berkeley, Los Alamos National Laboratories and Thomas Jefferson National Accelerator Facility. Each laboratory is assigned responsibility for accomplishing a well defined portion of the project's scope that takes advantage of their technical strengths: Argonne - Instruments; Brookhaven - Accumulator Ring; Lawrence Berkeley - Front End; Los Alamos – Normal conducting linac and RF power systems; TJNAF – Superconducting Linac; Oak Ridge - Target. Project execution is the responsibility of the SNS Project Director with the support of a central SNS Project Office at ORNL, which provides overall project management, systems integration, ES&H, quality assurance, and commissioning support. The SNS Project Director has authority for directing the efforts at all six partner laboratories and exercises financial control over all project activities. ORNL has subcontracted to an Industry Team that consists of an Architect-Engineer for the conventional facilities design and a Construction Manager for construction installation, equipment procurement, testing and commissioning support. Procurements by all six laboratories will be accomplished, to the extent feasible, by fixed price subcontracts awarded on the basis of competitive bidding.

## 6. Schedule of Project Funding

(dollars in thousands)

	Prior Year Costs	FY 2001	FY 2002	FY 2003	Outyears	Total
Project Cost						
Facility Cost <sup>1</sup>						
Line Item TEC .....	142,682	170,453	287,732	301,304	290,529	1,192,700
Plant Engineering & Design .....	0	0	0	0	0	0
Expense-funded equipment .....	0	0	0	0	0	0
Inventories .....	0	0	0	0	0	0
Total direct cost.....	142,682	170,453	287,732	301,304	290,529	1,192,700
Other project costs						
R&D necessary to complete project <sup>2</sup> .....	60,356	13,019	4,323	2,328	4,526	84,552
Conceptual design cost <sup>3</sup> .....	14,397	0	0	0	0	14,397
Decontamination & Decommissioning (D&D).....	0	0	0	0	0	0
NEPA Documentation costs <sup>4</sup> .....	1,948	0	0	0	0	1,948
Other project-related costs <sup>5</sup> .....	3,824	6,707	11,421	12,553	82,495	117,000
Capital equipment not related construction <sup>6</sup> .....	664	183	100	100	56	1,103
Total, Other project costs.....	81,189	19,909	15,844	14,981	87,077	219,000
Total project cost (TPC) .....	223,871	190,362	303,576	316,285	377,606	1,411,700

<sup>1</sup> Construction line item costs included in this budget request are for providing Title I and II design, inspection, procurement, and construction of the SNS facility for an estimated cost of \$1,192,700,000.

<sup>2</sup> A research and development program at an estimated cost of \$84,552,000 is needed to confirm several design bases related primarily to the accelerator systems, the target systems, safety analyses, cold moderator designs, and neutron guides, beam tubes, and instruments. Several of these development tasks require long time durations and the timely coupling of development results into the design is a major factor in detailed task planning.

<sup>3</sup> Costs of \$14,397,000 are included for conceptual design and for preparation of the conceptual design documentation prior to the start of Title I design in FY 1999.

<sup>4</sup> Estimated costs of \$1,948,000 are included to complete the Environmental Impact Statement.

<sup>5</sup> Estimated costs of \$117,000,000 are included to cover pre-operations costs.

<sup>6</sup> Estimated costs of \$1,103,000 to provide test facilities and other capital equipment to support the R&D program.

## 7. Related Annual Funding Requirements

(FY 2007 dollars in thousands)<sup>1</sup>

	Current Estimate	Previous Estimate
Facility operating costs .....	45,700	21,300
Facility maintenance and repair costs .....	24,800	25,300
Programmatic operating expenses directly related to the facility .....	40,000	22,500
Capital equipment not related to construction but related to the programmatic effort in the facility	11,800	2,100
GPP or other construction related to the programmatic effort in the facility .....	1,000	1,000
Utility costs .....	19,400	30,400
Accelerator Improvement Modifications (AIMs).....	7,300	4,100
<b>Total related annual funding (4Q FY 2006 will begin operations) .....</b>	<b>150,000</b>	<b>106,700</b>

During conceptual design of the SNS project, the annual funding requirements were initially estimated based on the cost of operating similar facilities (e.g. ISIS and the Advanced Photon Source) at \$106,700,000. The operating parameters, technical capabilities, and science program are now better defined and the key members of the ORNL team that will operate SNS are now in place. Based on these factors, the SNS Project developed a new estimate of annual operating costs, which was independently reviewed by the Department, and provides the basis of the current estimate indicated above. FY 2007 will be the first full year of operations and this estimate is generally representative of the early period of SNS operations. By the time SNS is fully instrumented and the facility is upgraded to reach its full scientific potential, the annual funding requirements will increase by an additional 10-15 percent.

## 8. Design and Construction of Federal Facilities

All DOE facilities are designed and constructed in accordance with applicable Public Laws, Executive Orders, OMB Circulars, Federal Property Management Regulations, and DOE Orders. The total estimated cost of the project includes the cost of measures necessary to assure compliance with Executive Order 12088, “Federal Compliance with Pollution Control Standards”; section 19 of the Occupational Safety and Health Act of 1970, the provisions of Executive Order 12196, and the related Safety and Health provisions for Federal Employees (CFR Title 29, Chapter XVII, Part 1960); and the Architectural Barriers Act, Public Law 90-480, and implementing instructions in 41 CFR 101-19.6. This project includes the construction of new buildings and/or building additions; therefore, a review of the GSA Inventory of Federal Scientific Laboratories is required. The project will be located in an area not subject to flooding determined in accordance with the Executive Order 11988.

<sup>1</sup> The previous estimate was in FY 2006 dollars.

# 02-SC-002 - Project Engineering Design (PED), Various Locations

(Changes from the FY 2002 Congressional Budget Request are denoted with a vertical line in the left margin.)

## 1. Construction Schedule History

	Fiscal Quarter				Total Estimated Cost (\$000)
	A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete	
FY 2002 Budget Request (Preliminary Estimate)	2Q 2002	3Q 2004	N/A	N/A	14,000
FY 2003 Budget Request (Current Estimate)	2Q 2002	3Q 2003	N/A	N/A	15,000 <sup>a</sup>

## 2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2002	3,000	3,000	3,000
2003	11,000	11,000	11,000
2004	1,000	1,000	1,000

## 3. Project Description, Justification and Scope

This PED request provides for Title I and Title II Architect-Engineering (A-E) services for Basic Energy Sciences (BES) projects related to the establishment of user centers for nanoscale science, engineering, and technology research. These funds allow designated projects to proceed from conceptual design into preliminary design (Title I) and definitive design (Title II). The design effort will be sufficient to assure project feasibility, define the scope, provide detailed estimates of construction costs based on the approved design and working drawings and specifications, and provide construction schedules including procurements. The design effort will ensure that construction can physically start or long-lead procurement items can be procured in the fiscal year in which Title III construction activities are funded.

Updated FY 2003 PED design projects are described below. Some changes may occur due to continuing conceptual design studies or developments prior to enactment of an appropriation. These changes will be reflected in subsequent years. Construction funding for one of the FY 2002 subprojects is also separately requested in FY 2003.

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<sup>a</sup> The full Total Estimated Cost (design and construction) ranges between \$239,000,000 - \$329,000,000. This estimate was based on conceptual data and should not be construed as a project baseline. Based on the results of peer review, the total design cost is changed to \$15,000,000. The full Total Estimated Cost for one project, subproject 02-04, currently proposed for construction is identified in the FY 2003 construction datasheet.

## Nanoscale Science Research Centers (NSRCs)

To support research in nanoscale science, engineering, and technology, the U.S. has constructed outstanding facilities for *characterization and analysis* of materials at the nanoscale. Most of these world-class facilities are owned and operated by BES. They include, for example, the synchrotron radiation light source facilities, the neutron scattering facilities, and the electron beam microscope centers. However, world-class facilities that are widely available to the scientific research community for nanoscale *synthesis, processing, and fabrication* do not exist. NSRCs are intended to fill that need. NSRCs will serve the Nation's researchers and complement university and industrial capabilities in the tradition of the BES user facilities and collaborative research centers. Through the establishment of NSRCs affiliated with existing major user facilities, BES will provide state-of-the-art equipment for materials synthesis, processing, and fabrication at the nanoscale in the same location as facilities for characterization and analysis. NSRCs will build on the existing research and facility strengths of the host institutions in materials science and chemistry research and in x-ray and neutron scattering. This powerful combination of colocated fabrication and characterization tools will provide an invaluable resource for the Nation's researchers.

In summary, the purposes of NSRCs are to:

- provide state-of-the-art nanofabrication and characterization equipment to in-house and visiting researchers,
- advance the fundamental understanding and control of materials at the nanoscale,
- provide an environment to support research of a scope, complexity, and disciplinary breadth not possible under traditional individual investigator or small group efforts,
- provide a formal mechanism for both short- and long-term collaborations and partnerships among DOE laboratory, academic, and industrial researchers,
- provide training for graduate students and postdoctoral associates in interdisciplinary nanoscale science, engineering, and technology research,
- provide the foundation for the development of nanotechnologies important to the Department.

Centers have been proposed by: Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), Lawrence Berkeley National Laboratory (LBNL), Oak Ridge National Laboratory (ORNL), and a consortium of Los Alamos National Laboratory (LANL) and Sandia National Laboratory (SNL). Based on peer review of the Center proposals, PED funding is being provided in FY 2002 and requested in FY 2003 for LBNL, ORNL, and LANL/SNL. Construction funding is also requested for ORNL in FY 2003.

FY 2002 Proposed Design Projects

FY 02-01: Center for Nanoscale Materials – Argonne National Laboratory

Fiscal Quarter				Total Estimated Cost (Design Only) (\$000)	Full Total Estimated Cost Projection <sup>a</sup> (\$000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
2Q 2002	2Q 2003	3Q 2003	N/A	2,000	45,000-65,000

Fiscal Year	Appropriations	Obligations	Costs
2002	0 <sup>b</sup>	0 <sup>b</sup>	0 <sup>b</sup>
2003	0 <sup>b</sup>	0 <sup>b</sup>	0 <sup>b</sup>

The Center for Nanoscale Materials (CNM) at ANL will consist of conventional facilities, fabrication facilities, characterization instruments, computational capabilities, and beamlines at the Advanced Photon Source (APS). The CNM will be attached to the APS at a location not occupied by one of the standard Laboratory-Office Modules that serve the majority of the APS sectors. Most specifications of the conventional facilities design for CNM will be intimately connected to the specifications of the technical systems. Towards this end, effort will be dedicated to optimizing both the conventional facilities and the technical facilities, looking for value engineering opportunities. The Center at Argonne will require approximately 10,000 square feet of class 1,000 clean room space for nanofabrication and characterization equipment. This facility will also require general purpose chemistry/biology laboratories (7,000 square feet) and electronic and physical measurement laboratories (3,000 square feet). To house the CNM staff, university collaborators (post docs, visiting students and faculty), and industry collaborators, approximately 16,000 square feet for offices and meeting rooms will be provided. The CNM is being coordinated with a State of Illinois effort. Based on the results of the FY 2001 peer review of the CNM, PED funding is not planned for FY 2002 or requested for this effort in FY 2003.

<sup>a</sup> The full TEC Projection (design and construction) is a preliminary estimate based on conceptual data and should not be construed as a project baseline.

<sup>b</sup> The FY 2002 Request included funding of \$1,000,000 in FY 2002 and FY 2003 for this project. Based on results of peer review, funding is not planned for FY 2002 or requested for this project in FY 2003.

02-02: The Molecular Foundry – Lawrence Berkeley National Laboratory

Fiscal Quarter				Total Estimated Cost (Design Only) (\$000)	Full Total Estimated Cost Projection <sup>a</sup> (\$000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
2Q 2002	3Q 2003	4Q 2003	N/A	8,300	55,000 – 75,000

Fiscal Year	Appropriations	Obligations	Costs
2002	500 <sup>b</sup>	500 <sup>b</sup>	500 <sup>b</sup>
2003	6,800 <sup>b</sup>	6,800 <sup>b</sup>	6,800 <sup>b</sup>
2004	1,000	1,000	1,000

The Molecular Foundry will be a two to four story high structure adjacent to the Advanced Light Source, with a total gross area of approximately 90,000 square feet and net usable area of approximately 53,000 square feet. Space in the new facility will support studies in nanostructures by providing offices and laboratories for materials science, physics, chemistry, biology, molecular biology and engineering, as well as approximately 6,000 square feet of high bay area. The building will be a state-of-the-art facility for the design, modeling, synthesis, processing, and fabrication of novel molecules and nanoscale materials and their characterization. State-of-the-art equipment will support this research; e.g.: cleanroom, class 10-100; controlled environment rooms; scanning tunneling microscopes; atomic force microscopes; transmission electron microscope; fluorescence microscopes; mass spectrometers; DNA synthesizer, sequencer; nuclear magnetic resonance spectrometer; ultrahigh vacuum scanning-probe microscopes; photo, uv, and e-beam lithography equipment; peptide synthesizer; advanced preparative and analytical chromatographic equipment; and cell culture facilities. New and existing beamlines at the ALS, not part of this PED activity, will support efforts at the Molecular Foundry.

<sup>a</sup> The full TEC Projection (design and construction) is a preliminary estimate based on conceptual data and should not be construed as a project baseline.

<sup>b</sup> The FY 2002 Request included \$1,000,000 for FY 2002 and \$2,000,000 for FY 2003. Based on the results of peer review, current funding plan is \$500,000 for FY 2002, \$6,800,000 for FY 2003, and \$1,000,000 for FY 2004.

02-03: Center for Functional Nanomaterials – Brookhaven National Laboratory

Fiscal Quarter				Total Estimated Cost (Design Only) (\$000)	Full Total Estimated Cost Projection <sup>a</sup> (\$000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
2Q 2002	3Q 2003	4Q 2003	N/A	3,000	45,000-65,000

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2002	0 <sup>b</sup>	0 <sup>b</sup>	0 <sup>b</sup>
2003	0 <sup>b</sup>	0 <sup>b</sup>	0 <sup>b</sup>

The Center for Functional Nanomaterials will include class 10 clean rooms, general laboratories, wet and dry laboratories for sample preparation, fabrication, and analysis. Included will be the equipment necessary to explore, manipulate, and fabricate nanoscale materials and structures. Also included are individual offices and landscape office areas, seminar area, transient user space for visiting collaborators with access to computer terminals, conference areas on both floors, and vending/lounge areas. In addition it will include circulation/ancillary space, including mechanical equipment area, toilet rooms, corridors, and other support spaces. Equipment procurement for the project will include equipment needed for laboratory and fabrication facilities for e-beam lithography, transmission electron microscopy, scanning probes and surface characterization, material synthesis and fabrication, and spectroscopy. The building will incorporate human factors into its design to encourage peer interactions and collaborative interchange by BNL staff and research teams from collaborating institutions. In addition to flexible office and laboratory space it will provide “interaction areas”, a seminar room and a lunch room for informal discussions. This design approach is considered state-of-the-art in research facility design as it leverages opportunities for the free and open exchange of ideas essential to creative research processes. Based on the results of the FY 2001 peer review of the Center for Functional Nanomaterials, PED funding is not planned for FY 2002 or requested for this project in FY 2003.

<sup>a</sup> The full TEC Projection (design and construction) is a preliminary estimate based on conceptual data and should not be construed as a project baseline.

<sup>b</sup> The FY 2002 Request included \$1,000,000 in FY 2002 and \$2,000,000 in FY 2003 for this project. Based on results of peer review, funding is not planned for FY 2002 or requested for this project in FY 2003.



02-04: Center for Nanophase Materials Sciences – Oak Ridge National Laboratory

Fiscal Quarter				Total Estimated Cost (Design Only) (\$000)	Full Total Estimated Cost Projection <sup>a</sup> (\$000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
2Q 2002 <sup>b</sup>	3Q 2003 <sup>b</sup>	4Q 2003 <sup>b</sup>	N/A	2,500 <sup>b</sup>	64,000

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2002	1,500 <sup>b</sup>	1,500 <sup>b</sup>	1,500 <sup>b</sup>
2003	1,000 <sup>b</sup>	1,000 <sup>b</sup>	1,000 <sup>b</sup>

A major focus of the Center for Nanophase Materials Sciences (CNMS) will be the application of neutron scattering for characterization of nanophase materials. In this area, CNMS will be a world leader. With the construction of the new Spallation Neutron Source (SNS) and the upgraded High Flux Isotope Reactor (HFIR), it is essential that the U.S.-based neutron science R&D community grow to the levels found elsewhere in the world and assume a scientific leadership role. Neutron scattering provides unique information about both atomic-scale structure and the dynamics of a wide variety of condensed matter systems including polymers, macromolecular systems, magnetic and superconducting materials, and chemically complex materials, particularly oxides and hydrogen-containing structures. Consequently, the intense neutron beams at HFIR and SNS will make, for the first time, broad classes of related nanoscale phenomena accessible to fundamental study.

The CNMS will occupy an 80,000 sq.ft. building containing wet and dry materials synthesis and characterization laboratories; clean rooms and materials imaging, manipulation, and integration facilities in a nanofabrication research laboratory; computer-access laboratories for nanomaterials theory and modeling; and office space for staff and visitors. The CNMS facility will consist of a multi-story building for materials synthesis and characterization contiguous with a single-story structure for nanofabrication having Class 100, Class 1,000, and Class 10,000 clean areas. The latter portion of the facility will be built using a construction approach that will meet low electromagnetic field, vibration, and acoustic noise requirements for special nanofabrication and characterization equipment. Based on the results of review, this project is now proposed for construction funding in FY 2003.

<sup>a</sup> The full TEC Projection (design and construction) in the FY 2002 PED datasheet is a preliminary estimate based on conceptual data. The TEC displayed above is the TEC displayed in the FY 2003 construction datasheet for this project (03-R-312).

<sup>b</sup> Funding of \$1,000,000 in FY 2003 and \$2,000,000 in FY 2004 was identified in the FY 2002 Request for this project. Based on the results of peer review, this project will be funded at \$1,500,000 in FY 2002 and \$1,000,000 in FY 2003.

02-06: The Center for Integrated Nanotechnologies (CINT) – Sandia National Laboratory

Fiscal Quarter				Total Estimated Cost (Design Only) (\$000)	Full Total Estimated Cost Projection <sup>a</sup> (\$000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		
1Q 2002	3Q 2003	4Q 2003	N/A	4,200	30,000 – 60,000

Fiscal Year	Appropriations	Obligations	Costs
2002	1,000 <sup>b</sup>	1,000 <sup>b</sup>	1,000 <sup>b</sup>
2003	3,200 <sup>b</sup>	3,200 <sup>b</sup>	3,200 <sup>b</sup>

The Center for Integrated Nanotechnologies (CINT), a Center jointly managed by the Los Alamos National Laboratory (LANL) and Sandia National Laboratory (SNL), has as its primary objective the development of the scientific principles that govern the performance and integration of nanoscale materials, thereby building the foundations for future nanotechnologies. CINT will consist of a main research facility to be located in an unrestricted area just outside the restricted area at Sandia National Laboratory (SNL) and two smaller “gateway” facilities located on the campuses of SNL and LANL. These gateways will provide office space and, in the case of the LANL gateway limited amounts of laboratory space, for researchers who need access to specialized facilities located on these campuses. The SNL gateway will use existing space in SNL’s Integrated Materials Research Laboratory; the LANL gateway will require construction of a small building. The CINT gateway to SNL will focus on specialized microfabrication and nanomaterials capabilities and expertise. The CINT gateway to LANL will focus on connecting CINT researchers to the extensive biosciences and nanomaterials capabilities at LANL. The main research facility and the gateways will be managed as one integrated facility by a single management structure. The CINT will focus on nanophotonics, nanoelectronics, nanomechanics, and functional nanomaterials. The Center will make use of a wide range of specialized facilities, including the Los Alamos Neutron Science Center and the National High Magnetic Field Laboratory at LANL; the Microelectronics Development Laboratory and the Compound Semiconductor Research Laboratory at SNL.

The main CINT building in Albuquerque will provide an open environment readily accessible by students and visitors, including foreign nationals. This structure will house state-of-the-art clean rooms and equipment for nanolithography, atomic layer deposition, and materials characterization along with general purpose chemistry and electronics labs and offices for Center staff and collaborators.

<sup>a</sup> The full TEC Projection (design and construction) is a preliminary estimate based on conceptual data and should not be construed as a project baseline. CINT combines the projects identifies as the “Synthesis and Characterization Laboratory” at LANL and the “Nanofabrication and Integration Laboratory” at SNL described separately in FY 2002.

<sup>b</sup> The FY 2002 Request included a total of \$1,000,000 in FY 2002 and \$2,000,000 in FY 2003 for the LANL and SNL components of this combined project. Based on results of peer review, current PED funding plan for the combined project is \$1,000,000 for FY 2002 and \$3,200,000 FY 2003.

The complex will require class 1,000 clean room space for nanofabrication and characterization equipment and an additional class 100 clean room space for lithography activities. This facility will also require general purpose chemistry/biology laboratories and electronic and physical measurement laboratories. To house the Center staff, collaborators, Center-sponsored post docs, visiting students and faculty, and industry collaborators, offices and meeting rooms will be provided.

#### 4. Details of Cost Estimate <sup>a</sup>

Design Phase	(dollars in thousands)	
	Current Estimate	Previous Estimate
Preliminary and Final Design costs (Design Drawings and Specifications) .....	11,250	10,500
Design Management costs (15% of TEC) .....	2,250	2,100
Project Management costs (10% of TEC) .....	1,500	1,400
Total Design Costs (100% of TEC) .....	15,000	14,000
Total, Line Item Costs (TEC).....	15,000	14,000

#### 5. Method of Performance

Design services will be obtained through competitive and/or negotiated contracts. M&O contractor staff may be utilized in areas involving security, production, proliferation, etc. concerns.

#### 6. Schedule of Project Funding

	(dollars in thousands)					Total
	Prior Year Costs	FY 2001	FY 2002	FY 2003	Outyears	
Facility Cost.						
PED.....	0	0	3,000	11,000	1,000	15,000
Other project costs						
Conceptual design cost.....	0	1,155	0	0	0	1,155
NEPA documentation costs.....	0	0	0	0	0	0
Other project related costs .....	0	0	0	0	0	0
Total, Other Project Costs.....	0	1,155	0	0	0	1,155

<sup>a</sup> This cost estimate is based on direct field inspection and historical cost estimate data, coupled with parametric cost data and completed conceptual studies and designs when available. The cost estimate includes design phase activities only. Construction activities will be requested as individual line items on completion of Title I design. The annual escalation rates assumed in the FY 2002 estimate for FY 2002 and FY 2003 are 3.3 and 3.4 percent, respectively.

(dollars in thousands)

	Prior Year Costs	FY 2001	FY 2002	FY 2003	Outyears	Total
Conceptual design cost.....	0	1,155	0	0	0	1,155
NEPA documentation costs.....	0	0	0	0	0	0
Other project related costs .....	0	0	0	0	0	0
Total, Other Project Costs .....	0	1,155	0	0	0	1,155

# 03-SC-002, Project Engineering Design (PED), Stanford Linear Accelerator Center

## 1. Construction Schedule History

	Fiscal Quarter				Total Estimated Cost <sup>1</sup> (\$000)
	A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Project Complete	
FY 2003 Budget Request (Preliminary Estimate)	1Q FY2003	2Q FY2005	1Q FY2004	4Q FY2006	\$33,500

## 2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
2003	6,000	6,000	5,500
2004	15,000	15,000	15,500
2005	10,000	10,000	10,000
2006	2,500	2,500	2,500

## 3. Project Description, Justification and Scope

These funds allow designated projects to proceed from conceptual design into preliminary design (Title I) and definitive design (Title II). The design effort will be sufficient to assure project feasibility, define the scope, provide detailed estimates of construction costs based on the approved design and working drawings and specifications, and provide construction schedules including procurements. The design effort will ensure that construction can physically start or long-lead procurement items can be procured in the fiscal year in which Title III construction activities are funded.

The FY 2003 Request is for the Linac Coherent Light Source (LCLS) Project to be located at the Stanford Linear Accelerator Center (SLAC).

The purpose of the LCLS Project is to provide laser-like radiation in the x-ray region of the spectrum that is 10 orders of magnitude (i.e., a factor of 10,000,000,000) greater in peak power and peak brightness than any existing coherent x-ray light source. This advance in brightness is similar to that of a synchrotron over a 1960's laboratory x-ray tube. Synchrotrons revolutionized science across disciplines ranging from atomic physics to structural biology. Advances from the LCLS are expected to

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<sup>1</sup> The full TEC Projection (design and construction) ranges between \$165,000,000 and \$225,000,000. This is a preliminary estimate based on conceptual data and should not be construed as a project baseline.

be equally dramatic. The LCLS Project will provide the first demonstration of an x-ray free-electron-laser (FEL) in the 1.5 – 15 Å range and will apply these extraordinary, high-brightness x-rays to an initial set of scientific problems. This will be the world's first such facility.

The LCLS is based on the existing SLAC linac. The SLAC linac can accelerate electrons or positrons to 50 GeV for colliding beams experiments and for nuclear and high-energy physics experiments on fixed targets. At present, the first two-thirds of the linac is being used to inject electrons and positrons into PEP-II, and the entire linac is used for fixed target experiments. When the LCLS is completed, this latter activity will be limited to 30 percent of the available beam time and the last one-third of the linac will be available for the LCLS a minimum of 70 percent of the available beam time. For the LCLS, the linac will produce high-brightness 5 - 15 GeV electron bunches at a 120 Hz repetition rate. When traveling through the 120 meter long LCLS undulator, these electron bunches will amplify the emitted x-ray radiation to produce an intense, coherent x-ray beam for scientific research.

The LCLS makes use of technologies developed for the SLAC and the next generation of linear colliders, as well as the progress in the production of intense electron beams with radio-frequency photocathode guns. These advances in the creation, compression, transport, and monitoring of bright electron beams make it possible to base this next generation of x-ray synchrotron radiation sources on linear accelerators rather than on storage rings.

The LCLS will have properties vastly exceeding those of current x-ray sources (both synchrotron radiation light sources and so-called “table-top” x-ray lasers) in three key areas: peak brightness, coherence (i.e., laser like properties), and ultrashort pulses. The peak brightness of the LCLS is 10 orders of magnitude greater than current synchrotrons, providing  $10^{12}$ - $10^{13}$  x-ray photons in a pulse with duration of 230 femtoseconds. These characteristics of the LCLS will open new realms of scientific applications in the chemical, material, and biological sciences. The LCLS Scientific Advisory Committee, working in coordination with the broad scientific community, identified high priority initial experiments that are summarized in the document, *LCLS: The First Experiments*. These first five areas of experimentation are fundamental studies of the interaction of intense x-ray pulses with simple atomic systems, use of the LCLS to create warm dense matter and plasmas, structural studies on single nanoscale particles and biomolecules, ultrafast dynamics in chemistry and solid-state physics, and studies of nanoscale structure and dynamics in condensed matter.

The experiments fall into two classes. The first follows the traditional role of X-rays to probe matter without modifying it while the second utilizes the phenomenal intensity of the LCLS to excite matter in fundamentally new ways and to create new states in extreme conditions. The fundamental studies of the interactions of intense X-rays with simple atomic systems are necessary to lay the foundation for all interactions of the LCLS pulse with atoms embedded in molecules and condensed matter. The structural studies of individual particles or molecules make use of recent advances in imaging techniques for reconstructing molecular structures from diffraction patterns of non-crystalline samples. The enormous photon flux of the LCLS makes it feasible to determine the structure of a *single* biomolecule or small nanocrystal using only the diffraction pattern from a single moiety. This application has enormous potential in structural biology, particularly for important systems such as membrane proteins, which are virtually uncharacterized by X-ray crystallography because they are nearly impossible to crystallize. The last two sets of experiments make use of the extremely short pulse of the LCLS to follow dynamical

processes in chemistry and condensed matter physics in real time. The use of ultrafast X-rays will open up whole new regimes of spatial and temporal resolution to both techniques.

The proposed LCLS Project requires a 150 MeV injector to be built at Sector 20 of the 30-sector SLAC linac to create the electron beam required for the x-ray FEL. The last one third of the linac will be modified by adding two magnetic bunch compressors. Most of the linac and its infrastructure will remain unchanged. The existing components in the Final Focus Test Beam tunnel will be removed and replaced by a new 120 meter undulator and associated equipment.

#### 4. Details of Cost Estimate<sup>1</sup>

Design Phase	(dollars in thousands)	
	Current Estimate	Previous Estimate
Preliminary and Final Design costs (Design Drawings and Specifications) .....	25,125	N/A
Design Management costs (15% of TEC) .....	5,025	N/A
Project Management costs (10% of TEC) .....	3,350	N/A
Total Design Costs (100% of TEC) .....	33,500	N/A
Total, Line Item Costs (TEC).....	33,500	N/A

#### 5. Method of Performance

A Conceptual Design Report (CDR) for the project will be completed and reviewed prior to beginning this work. Key design activities will be identified in the areas of the injector, undulator, x-ray optics and experimental halls that will reduce the risk of the project and accelerate the startup. Also, the management systems for the project will be put in place and proven during the Project Engineering Design (PED) phase. These activities will be managed by an LCLS project office in the Stanford Synchrotron Radiation Laboratory (SSRL) Division of SLAC. Portions of the project will be executed by staff at Argonne National Laboratory (ANL) and Lawrence Livermore National Laboratory (LLNL).

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<sup>1</sup> This cost estimate includes design phase activities only. Construction activities will be requested to be funded in FY 2004.

## 6. Schedule of Project Funding

(dollars in thousands)

	Prior Year Costs	FY 2001	FY 2002	FY 2003	Outyears	Total
Facility Cost						
PED .....	0	0	0	5,500	28,000	33,500
Other project costs						
Conceptual design cost .....	0	0	1,500	0	0	1,500
NEPA documentation costs .....	0	0	0	0	0	0
Other project related costs.....	0	0	0	0	0	0
Total, Other Project Costs .....	0	0	1,500	0	0	1,500
Total Project Cost (TPC) .....	0	0	1,500	5,500	28,000	35,000



# 03-R-312, Center For Nanophase Materials Sciences Oak Ridge National Laboratory, Oak Ridge, Tennessee

## 1. Construction Schedule History

Fiscal Quarter				Total Estimated Cost (\$000)	Total Project Cost (\$000)
A-E Work Initiated	A-E Work Completed	Physical Construction Start	Physical Construction Complete		

FY 2003 Budget Request (Preliminary Estimate) .....	2Q2002	1Q2003	3Q2003	4Q2006	\$64,000	\$65,000
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## 2. Financial Schedule

(dollars in thousands)

Fiscal Year	Appropriations	Obligations	Costs
<b>Project Engineering &amp; Design (PED)</b>			
2002	1,500 <sup>a</sup>	1,500 <sup>a</sup>	1,500 <sup>a</sup>
2003	1,000 <sup>a</sup>	1,000 <sup>a</sup>	1,000 <sup>a</sup>
<b>Construction</b>			
2003	24,000 <sup>a</sup>	24,000 <sup>a</sup>	14,000 <sup>a</sup>
2004	20,000	20,000	20,000
2005	17,500	17,500	21,500
2006	0	0	6,000

<sup>a</sup> Funding of \$1,000,000 in FY 2003 and \$2,000,000 in FY 2004 was identified in the FY 2002 President's Request for this project. Based on the results of peer review, this project is now proposed for PED funding of \$1,500,000 in FY 2002 and \$1,000,000 in FY 2003 and construction funding of \$24,000,000 in FY 2003.

### **3. Project Description, Justification and Scope**

This proposed Center for Nanophase Materials Sciences (CNMS) will establish a nanoscale science research center at Oak Ridge National Laboratory (ORNL) that will integrate nanoscale science research with neutron science, synthesis science, and theory/modeling/simulation of nanophase materials, bringing together four areas where the United States has clear national research needs. The total gross area of the new building will be approximately 80,000 square feet, providing state-of-the-art clean rooms, and general laboratories for sample preparation, fabrication and analysis. Included will be initial equipment for nanoscale materials research such as surface analysis equipment, nanofabrication facilities, etc. The facility, collocated with the Spallation Neutron Source complex, will house ORNL staff members and visiting scientists from academia and industry. There are no existing buildings at ORNL that could serve these needs.

The CNMS's major scientific thrusts will be in nano-dimensional soft materials, complex nanophase materials systems, and the crosscutting areas of interfaces and reduced dimensionality that become scientifically critical on the nanoscale. A major focus of the CNMS will be to exploit ORNL's unique facilities and capabilities in neutron scattering to determine the structure of nanomaterials, to develop a detailed understanding of synthesis and self-assembly processes in "soft" materials, and to study and understand collective (cooperative) phenomena that emerge on the nanoscale. Neutron scattering provides unique information (complementary to that provided by other methods) about both the atomic-scale structure and the dynamics of a wide variety of condensed matter systems including polymers, macromolecular systems, magnetic and superconducting materials, and chemically complex materials, particularly oxides and hydrogen-containing structures. The intense neutron beams available at the upgraded High Flux Isotope Reactor and the new Spallation Neutron Source will make broad classes of related nanoscale phenomena accessible to fundamental study.

Since the late 1980s, there has been a recognized need to enhance U.S. capabilities in the synthesis of materials. These concerns are exacerbated by the challenges of controlled synthesis of nanophase materials. There is currently a critical, unmet national need for the synthesis of high quality nanophase research materials. It is also recognized that the existence of capabilities for science-driven synthesis of novel materials has played a central role in some of the most spectacular recent discoveries of new phenomena, including high-temperature superconductivity, the quantum and fractional quantum Hall effects, conducting polymers, and colossal magnetoresistance. Therefore, synthesis and characterization of nanophase materials (including copolymers and macromolecular systems, multilayered nanostructures, ceramics, composites, and alloys with nanoscale spatial, charge, and/or magnetic ordering) will be an essential component of the CNMS. With these capabilities the CNMS will become a national resource for nanophase materials for use by researchers across the nation.

The scope of this project is to construct the Center for Nanophase Materials Sciences. The engineering effort includes preliminary and final design. The project also includes procurement of experimental capital equipment and construction of facilities. While no FY 2002 PED funds were identified for this project on the FY 2002 PED Project Data Sheet (02-SC-002, Project Engineering Design (PED), various locations), SC plans to allocate FY 2002 and FY 2003 PED funding to complete design of the CNMS. FY 2003 construction funding will be used to initiate construction and equipment procurement.

## 4. Details of Cost Estimate<sup>1</sup>

	(dollars in thousands)	
	Current Estimate	Previous Estimate
Design Phase		
Preliminary and Final Design Costs.....	1,700	N/A
Design and Project Management Costs .....	300	N/A
Total, Design Costs.....	2,000	N/A
Construction Phase		
Improvements to Land .....	500	N/A
New Building and Additions .....	19,700	N/A
Special Equipment <sup>2</sup> .....	26,000	N/A
Utilities .....	500	N/A
Inspection, design and project liaison, testing, checkout and Acceptance .....	1,800	N/A
Construction and Project Management.....	1,700	N/A
Total, Construction Costs.....	50,200	N/A
Contingency (23.5% of Construction Costs) <sup>3</sup> .....	11,800	N/A
Total, Line Item Costs .....	64,000	N/A
Less: Non-Agency Contribution .....	0	N/A
Total, Line Item Costs (TEC).....	64,000	N/A

<sup>1</sup> The annual escalation rates are: FY 2002 – 2.6%, FY 2003 – 2.8%, FY 2004 – 2.8%, FY 2005 – 2.9% and FY 2006 – 2.9% as directed by DOE.

<sup>2</sup> Initial research equipment.

<sup>3</sup> Percent of TEC includes contingency for special equipment in the calculation.

## 5. Method of Performance

Design will be performed by an architect-engineer utilizing a fixed price subcontract. Construction will be performed by a fixed-price construction contractor administered by the ORNL operating contractor. Procurement of research capital equipment will be performed by the ORNL operating contractor. Project and construction management, inspection, coordination, utility tie-ins, testing and checkout witnessing, and acceptance will be performed by the ORNL operating contractor.

## 6. Schedule of Project Funding

	Prior Years	FY 2002	FY 2003	FY 2004	FY 2005	FY 2006	Total
Project Cost							
Facility Cost							
Design .....	0	1,500	1,000	0	0	0	2,500
Construction .....	0	0	14,000	20,000	21,500	6,000	61,500
Total, Line item TEC .....	0	1,500	15,000	20,000	21,500	6,000	64,000
Other project costs							
Conceptual design costs....	150	0	0	0	0	0	150
NEPA documentation Costs .....	5	0	0	0	0	0	5
Other project related Costs <sup>1</sup> .....	0	220	100	250	175	100	845
Total, Other Project Costs .....	155	220	100	250	175	100	1,000
Total Project Cost .....	155	1,720	15,100	20,250	21,675	6,100	65,000
Less: Non-Agency Contribution ..	0	0	0	0	0	0	0
Total, Project Cost (TPC) .....	155	1,720	15,100	20,250	21,675	6,100	65,000

<sup>1</sup> Experimental research will begin at the time of beneficial occupancy of the facility. These research costs are not part of the TPC and are funded by the BES subprograms.

## 7. Related Annual Funding Requirements

(FY 2006 dollars in thousands)

	Current Estimate	Previous Estimate
Annual facility operating costs .....	\$18,000	N/A
Total related annual funding .....	TBD	N/A
Total operating costs (operating from FY 2006 through FY 2055) .....	TBD	N/A

## **8. Design and Construction of Federal Facilities**

All DOE facilities are designed and constructed in accordance with applicable Public Laws, Executive Orders, OMB Circulars, Federal Property Management Regulations, and DOE Orders. The total estimated cost of the project includes the cost of measures necessary to assure compliance with Executive Order 12088, "Federal Compliance with Pollution Control Standards"; section 19 of the Occupational Safety and Health Act of 1970, the provisions of Executive Order 12196, and the related Safety and Health provisions for Federal Employees (CFR Title 29, Chapter XVII, Part 1960); and the Architectural Barriers Act, Public Law 90-480, and implementing instructions in 41 CFR 101-19.6. This project will be located in an area not subject to flooding determined in accordance with the Executive Order 11988. DOE has reviewed the U.S. General Services Administration (GSA) inventory of Federal Scientific laboratories and found insufficient space available, as reported by the GSA inventory.